XSEDE

eXtreme Science and Engineering Discovery Environment

2012 Q4: October 1, 2012, through December 31, 2012

XSEDE Senior Management Team

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Janet Brown (PSC)	Manager of Systems and Software Engineering
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Carol Song (PU)	Chair of the XD Service Providers Forum

XSEDE QUARTERLY REPORT

Contents

1 Overview

The Extreme Science and Engineering Discovery Environment (XSEDE) is the most advanced, powerful, and robust collection of integrated digital resources and services in the world. It is an integrated cyberinfrastructure ecosystem with singular interfaces for allocations, support, and other key services that researchers can use to interactively share computing resources, data, and expertise.

1.1 Project Context

Scientists, engineers, social scientists, and humanities experts around the world—many of them at colleges and universities—use advanced digital resources and services every day. Computational technologies and resources such as supercomputers, visualization systems, storage systems and collections of data, software, and networks are critical to the success of those researchers, who use them to advance our understanding of our world, and to make our lives healthier, safer, and better. XSEDE integrates these resources and services, makes them easier to use, and helps more people use them. XSEDE currently supports 16 supercomputers and high-end visualization and data analysis resources across the country.

Digital services, meanwhile, provide users with seamless integration to NSF's high-performance computing and data resources. XSEDE's integrated, comprehensive suite of advanced digital services is developing and implementing tools, methods, and policies to federate with other high-end facilities and with campus-based resources, serving as the foundation for a national cyberinfrastructure ecosystem. Common authentication and trust mechanisms, global namespace and filesystems, remote job submission and monitoring, and file transfer services are examples of XSEDE's advanced digital services. XSEDE's distributed systems architecture allows open development for future digital services and enhancements.

XSEDE also provides the expertise to ensure that researchers can effectively use the supercomputers and tools. Those include:

- Extended Collaborative Support that includes teaming with individual research groups or with research communities to extend their capabilities.
- An advanced hardware and software architecture rooted in user requirements and hardened by systems engineering that allows for individualized user experiences, consistent and enduring software interfaces, improved data management, and ways for campus resources to be transparently integrated into the overall XSEDE infrastructure.
- The XSEDE User Portal, a web interface that allows users to monitor and access XSEDE resources, manage jobs on those resources, report issues, and analyze and visualize results.
- Coordinated allocations of NSF's high-end resources and digital services.
- A powerful and extensible network, in which each XSEDE service provider is connected to a Chicago-based hub at 10 gigabits per second and has a second 10 gigabit-per-second connection to another national research and education network.
- Specialized community-provided services that serve a particular function and allow for rapid innovation and experimentation.
- Advanced cybersecurity to ensure that XSEDE resources and services provide confidentiality, integrity and availability of information
- Training, Education, and Outreach efforts that expand the scope and scale of activities to foster greater community participation in XSEDE-based projects through curriculum development, live and web-based training offerings, outreach at professional society meetings, and engagement of under-represented faculty and students.

- Advanced support for novel and innovative projects.
- A fellowship program that brings Campus Champions working closely with Extended Collaborative Support Service staff on user identified challenges for up to a year.
- The Technology Insertion Service, which allows researchers to recommend technologies for inclusion in the XSEDE infrastructure and enables the XSEDE team to evaluate those technologies and incorporate them where appropriate.

1.1.1 Communities Served

The national, and global, user community that relies on XSEDE for HPC resources has grown tremendously. XSEDE continued to see increased HPC resource user numbers in Q4 2012, with 644 new users added in the quarter. The number of open individual accounts was at 6,464, and the number of non-gateway individuals charging jobs reached a new high at 2,229. An additional 1,629 users submitted jobs via science gateways—also a new high with over 40% of XSEDE users submitting jobs via gateways. Counting current individual accounts and gateway users together, the XSEDE community numbered 8,093 users.

Further details can be found Appendix E.

1.1.2 XSEDE's Integrated, Distributed Environment

XSEDE is taking on the difficult but necessary task of documenting a clearly specified architectural design for its distributed systems architecture. Given the nature of the end game of the proposal competition that ultimately resulted in the XSEDE award, the project has had to substantially redesign the architecture originally proposed in order to incorporate innovative and important elements of the previously competing proposal. While this has been difficult and has led to some confusion, the project is making progress in this area and will begin to produce design documents that specify the architecture in detail during the coming months.

1.1.3 Project Governance

The XSEDE project has established an organizational structure and governance that promotes efficient and effective project performance. As this is a distributed project involving 17 partner institutions and with many other stakeholders including NSF, and thousands of users, it was necessary to establish a governance model that balances efficiency and inclusiveness. The XSEDE governance model has strong central management to provide rapid response to issues and opportunities, delegation and decentralization of decision-making authority, openness to genuine stakeholder participation, and improved professional project management practices including formal risk management and change control.

The XSEDE governance model is geared towards inclusion of, and responsiveness to, users, service providers, and the NSF scientific community. The various stakeholders have input through three distinct advisory bodies, which have direct access to the XSEDE Project Director and the XSEDE senior management team through regularly scheduled meetings. In order to remain well informed of the requirements of the user community, XSEDE leadership receives advice and counsel from the User Advisory Committee, the XD Service Providers Forum, the XSEDE Advisory Board, and the TEOS Advisory Committee. These advisory committees are intimately involved with XSEDE management in guiding the project towards optimal operations, service, and support for users.

The XSEDE project is managed by a senior management team consisting of the PI/Project Director as chair, the co-PIs and key leaders of major areas of the XSEDE project, the Chair of the User Advisory Committee, and the Chair of the XD Service Providers Forum. This team is constituted from those responsible for the day-to-day operation of the project and is the highest-level management body in the organization. In order to be responsive to both the user community and the set of Service Providers with whom we will collaborate, the chairs of the User Advisory Committee and the XD Service Providers Forum are members of this team.

1.2 Project Highlights

At the close of the second quarter of the second year of XSEDE, the project has gone beyond the initial growing pains and find its stride in many areas across the project. We are now looking to optimize many processes to enhance our efficiency is our operations and support across the project. Overall progress is quite good with some exceptions noted in the details in various sections of this report. This is clearly evidenced by the regular reporting of science and engineering success XSEDE has supported and enabled. In Section 2 of this report you will note a few of them we have highlighted this quarter that are very high-impact science or engineering research.

The SC12 conference in Salt Lake City, Utah and the XSEDE exhibit along with the Annual Highlights book were major accomplishments for the project this quarter. The booth saw many attendees coming to find out more about XSEDE and was the nexus for many new connections with the community.

The Campus Bridging activity has been moving forward with renewed vigor with the bulk of efforts in the area of moving the GFFS Pilot project forward and in the software packaging projects. One report describing priorities for Campus Bridging in years 2-5 was published, and a detailed plan for cluster software distribution was drafted and disseminated within XSEDE for comment.

XSEDE continues its high level of support of researchers with our Extended Collaborative Support Services (ECSS) staff engaged in 85 active projects during this past quarter covering a variety of areas. Unfortunately, our User Survey indicates only 28% of users were aware of ECSS. External Relations is now working to publicize ECSS more widely. We are also working to allow users to post their own brief write-ups of achievements which XSEDE has enabled. This will include how XSEDE has helped them achieve their research goals. The use of science gateways continues to grow with gateway usage posting a new high in the number of researchers accessing XSEDE resources via gateways at 1,629.

XSEDE User Services continues to provide high quality support for the community in a variety of ways. The XSEDE Resource Allocations Committee 427M Service Units of 1.1B Service Units requested, including awards on the new Stampede system. Our first multi-site course, this one on OpenACC, reached over 8000 attendees (in person, and online), was very successful and seems to be a model for broad training impact on the community. We are developing plans for several of these to be offered during calendar 2013. User support tickets continued to be resolved and mined for patterns, revealing that storage systems, data transfers, and availability of specific software packages are the current top issues documented in user tickets. The second user survey was initiated, incorporating lessons learned from the initial survey. User documentation continued to expand with new documents covering Stampede and the BigJobs community code. The XSEDE User Portal continued to improve existing features such as the change password procedure, and add new capabilities including *add user* (to an allocation). In addition, several 'project' activities are making progress and should complete in CY2013. The new ticket system is being deployed, the training certification process is advancing, a new mobile device web interface is being developed, and the storage allocations process should be implemented before the end of Project Year 2.

Training continues to be very effective reaching over 8,000 users and potential users in this quarter period via in-person, online, and webcast training workshops. Fifteen scheduled events took place, including a large multi-site simulcast course on OpenACC. The next quarter will be an exceptionally busy one, with Stampede training ramping up as well as a number of other activities. Nineteen training events are already scheduled for next quarter.

Planning for the XSEDE’13 conference has ramped up this past quarter with many of the early planning for submissions, web site, logistics and related activities being completed. Numerous XSEDE staff, Campus Champions and members of the community are members of the XSEDE13 Conference planning committee. We have been very pleased by the number of members of the larger community volunteering time and effort toward this important event. The committee is developing very exciting plans for the Conference to be held July 22-25.

From and XSEDE Operations perspective, we have begun to put in place a series of new capabilities to enhance productivity for our researchers. Work began to implement storage allocations within the XSEDE allocations process, POPS, and service provider accounting systems. Detailed configurations and pricing for the distributed hardware that will host the XSEDE-wide file system were finalized. Internet2 was selected to provide connectivity for XSEDE. Throughout the quarter, there were several planned and unplanned outages; however, the SysOps team maintained high overall uptime, which ensured data integrity and availability. Overall, we achieved 99.64% uptime for all but one of the production central services (the Karnak service only has a 91.1% uptime) while fielding almost 2,100 tickets of which 35% were closed within 2 business days. During this time no security vulnerabilities were identified that required XSEDE-wide notification, and there were no known compromised user accounts and no security issues with XSEDE resources.

Our October 12, 2012 XSEDE Advisory Board teleconference had a focus on our Industry Relations Program. This discussion resulted in firm guidance about moving the area forward within the project and the development of a call for participation in an “XSEDE Industry Challege.” A plan for this will be developed once a Level 3 manager is identified including risks and resource usage.

TEOS Advisory Committee met via conference call on Thursday October 18, 2012. At the 90-minute meeting, TEOS managers presented their responses to the NSF Review, as well as the feedback from the AC meeting on their presentations at the previous meetings. The expanded membership brings in new perspectives, though it complicates finding dates that allow participation by all the committee members.

Based on advice from the TEOS Advisory Committee, the TEOS team conducted the first in a series of annual retreats. The retreat focused on improving integration of activities among the TEOS team and with the rest of XSEDE. The discussions are helping to understand and improve workflows among the various teams, and to improve communications internally and externally. We continued our work with several institutions on formal computational science programs and presented XSEDE education materials at two national forums – a meeting of the Coalition for Academic Scientific Computation (CASC) and SC12.

This is the first quarter in which we report with the Technology Investigation Service (TIS) fully integrated into the larger XSEDE project. TIS Project Management completed the Program Change Request (PCR) to formally and officially combine TIS and XSEDE. The evaluation process is continuing to identify and evaluate technologies that might be useful in XSEDE. In addition, TIS has begun engaging other areas of XSEDE. In particular, the Operations group and the SD&I teams and have identified a technology evaluation that will complement work being done in the Operations and SD&I teams, and reached agreement on how to better integrate the provisioning of test systems for evaluations across all three groups.

Our Systems and Software Engineering (S&SE) activities are now becoming more routine and manageable to the benefit of the project. S&SE has become more efficient in its ongoing efforts to identify and elicit new user needs and capabilities and in assisting in the development of Use Cases with the Architecture & Design (A&D) team and key stakeholders. The S&SE, A&D and in collaboration with major stakeholders, has focused on developing a large number of Use Cases previously identified as priorities in the project in order to both to optimize the Use Case Development process and to allow a global prioritization of Use Cases once a large number have been documented. This will allow us to deliver the highest value Use Cases sooner.

The Software Development and Integration (SD&I) has also been making great progress working to close out the remaining 5 of the original 100 activities planned as part of "*Increment 2*" and initiating 16 activities prioritized by the User Requirements and Prioiritization Working Group for "*Increment 3*." This was the first instance of fully utilizing our prioritization process to guide the activities of SD&I.

2 Science and Engineering Highlights

2.1 Biophysics: Large-scale molecular dynamics simulations of anesthetic effects on ion channels (Pei Tang, University of Pittsburgh School of Medicine)

Anesthetics work by interfering with aspects of neurotransmission. One example is inhibiting or promoting the passage of ions through channels in the cell walls. Pentameric ligand gated ion channels (pLGICs) are a family of structurally similar cationic and anionic channels involved in neurotransmission. GLIC is a prokaryotic cationic pLGIC. Potential of mean force (PMF) calculations predict that four specific mutations of GLIC, transforming it into GLIC4, converts the channel from Na^+ to highly Cl^- permeable (see figure). Measurements in *Xenopus* oocytes expressing GLIC4 showed that GLIC4 had indeed become anion selective, with an 18-fold preference for Cl^- ions over Na^+ ions (see figure). Furthermore, the functional measurements showed that GLIC4 became insensitive to the anesthetics propofol and etomidate as well as the channel blocker picrotoxin, while GLIC is not. Molecular dynamics (MD) simulations revealed why. Propofol binding to an intra-subunit site of GLIC shifted the tilting angles of the pore-lining helix TM2 towards closure at the hydrophobic gate region, resulting in different pore radius and hydration profiles, consistent with propofol inhibition of GLIC. In contrast, the pore of GLIC4 was much more resilient to perturbation from propofol binding. The combined computational and experimental studies underscore the importance of pore dynamics and conformation to anesthetic effects on channel functions.

Each simulation system contains ~168,000 atoms. The PMF and MD simulations were performed using the NAMD package [1,2] on XSEDE resources. Blacklight, Kraken and Ranger were used alternatively depending on availability of each machine at the time of the job submission. Although the NAMD package has been well optimized for calculations like this, the research progress has benefited from advice on minimizing queue-waiting times at each XSEDE site.

This work has been published in the Biochemical Journal; see Tillman, T. S., Cheng, M. H.,

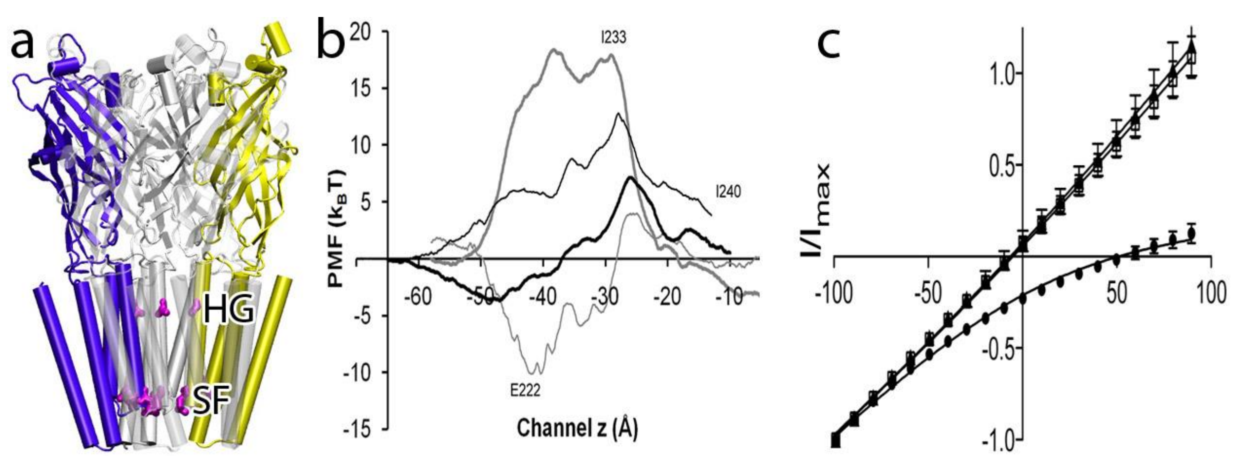

Figure 2.1.1. (**a**) Crystal structure of GLIC showing three mutations at the selectivity filter (SF) and one at the hydrophobic gate (HG). The mutant is named GLIC4. (**b**) Comparison of MD−calculated single ion PMFs for transporting Cl^- (thick lines) or Na^+ (thin lines) ion along the channel centerline of GLIC4 (black) and wild type GLIC (gray). (**c**) Reversal-potential measurements in *Xenopus* oocytes expressing GLIC4 show that GLIC4 is selective for Cl^-. Asymmetric IV curves for GLIC4 with 130 mM NaCl (▲), choline chloride (□) and sodium gluconate (●) in the external solution. Error bars represent standard error, n=5. The 60 mV positive shift in reversal potential on replacement of chloride with gluconate is indicative of chloride selectivity.

Chen, Q., Tang, P. and Xu, Y. *Reversal of ion charge selectivity renders the pentameric ligand-gated ion channel GLIC insensitive to anesthetics*. *Biochem. J.* 2012 Dec 07; 449 (part 1), 61-68.

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2. Kale, L.; Skeel, R.; Bhandarkar, M.; Brunner, R.; Gursoy, A.; Krawetz, N.; Phillips, J.; Shinozaki, A.; Varadarajan, K.; Schulten, K. *Journal of Computational Physics* **1999**, *151*, 283.

2.2 Biochemistry: Evaluating and improving the performance of RNA force fields in molecular dynamics simulations (Thomas Cheatham, University of Utah College of Pharmacy)

Thomas Cheatham's group focuses on adjusting the parameters of RNA force fields to better fit either experimentally determined data (NMR, X-ray crystallography, and others) or highly accurate quantum mechanical data. Making such comparisons, the group has identified potentially anomalous simulated conformations of the RNA molecule's sugar ring. Adjusting the force field parameters provided a better match with the quantum mechanical results and thus improved simulation accuracy, enhancing understanding of this biologically pivotal molecule and offering the potential for future therapeutic targets. These quantum calculations are extremely memory intensive, and the Blacklight machine at PSC was critical for performing them due to its large shared memory capability. The group's current work, testing these results in realistic molecular dynamic simulations of RNA, require simulating on long enough timescales for the RNA to convert between various conformations. Simulations of several microseconds of real time are necessary. To mitigate the months of traditional CPU hardware time that would otherwise be needed, the investigators have performed GPU-accelerated molecular dynamics on the NICS Keeneland machine. An alternative to long timescale simulations, enhanced sampling methods via replica exchange molecular dynamics, employs an ensemble of simulations (typically 10-50) run simultaneously at different temperatures and exchanging at defined intervals. They found that a special variant of replica exchange, called "reservoir replica exchange", works best for studying a small oligonucleotide. In this variant, a high temperature reservoir of structures is pre-generated using a conventional MD on a GPU. This reservoir is then coupled to the replica exchange procedure and drives convergence much faster than "regular" replica exchange They are now using the method to test new force fields and solvation conditions. The computational demands of this work would not have been achievable without allocations on Kraken at NICS, Ranger at TACC, and Gordon at SDSC.

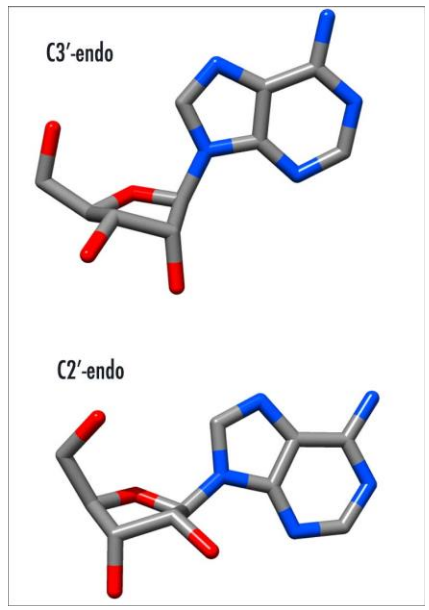


Figure 2.2.1 The Cheatham group's work revealed that some simulations inaccurately predicted which of two conformations the sugar moiety in RNA would take: C3'-endo (top) or C2'-endo

2.3 Molecular and Cellular Biosciences: Simulations of DNA damage and repair processes (PI: Suse Broyde, New York University)

A person doesn't have to go far to find a polycyclic aromatic hydrocarbon (PAH). These carcinogen precursors are inhaled through automobile exhaust during the morning commute, are present in cigarette smoke, and are part of any barbequed meal. Once ingested or inhaled, the multi-ringed molecules are converted into reactive carcinogenic compounds that can bind to DNA, sometimes literally bending the double helix out of its normal shape, to form areas of damage called lesions. The damaged DNA can create errors in the genetic code during replication, which may cause cancer-initiating mutations. It is the job of the nuclear excision repair (NER) system to repair damage caused by PAH lesions by removing the segment of DNA where the lesion is bound and patching up the resulting gap. But some lesions are especially resistant to this repair machinery, making them more likely to cause mutations. A research team at New York University (NYU) has gained new insights into the ability of certain PAH-derived lesions to evade the DNA repair machinery. Suse Broyde, a biology professor at NYU, and her team turned to Longhorn, Lonestar and Ranger at TACC to create the simulations. They revealed the lesions caused by the most potent carcinogens were the most resistant to repair because the lesions themselves stabilized the DNA they damaged. This made it difficult for a certain repair protein to mark the lesion for repair. Their research was published earlier this year in the February 2012 issue of *Biochemistry* and further articles about NER and DNA lesions appeared in *Nucleic Acids Research* in July and August. The stability of the DNA double helix is a key feature that determines whether DNA is flagged for repair in the first place by a protein called XPC. The protein patrols the genome looking for weakened areas. When it finds weak spot, it slips a structure called a beta-hairpin between the strands, marking the DNA for NER. But if a lesion makes DNA more stable, the strands become more difficult to separate and the beta hairpin can't signal for repair. Broyde and her team examined six different lesions types (caused by three chemicals with two different geometric configurations each). The simulations revealed that those caused by dibenzo[a,l]pyrene, the most tumorigenic PAH investigated, were the most resistant to repair. The five-ringed structure of the carcinogen provided ample stacking opportunities, which stabilized the DNA much better than the four and three-ringed structures of the other PAHs that were examined. Knowing which lesions are the most repair-resistant could play an important role in preventative medicine, said Broyde, as individuals harboring them could be counseled to avoid further exposure, particularly in the case of smokers.

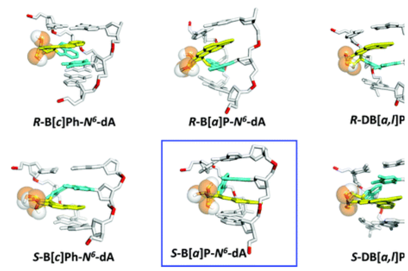


Figure 2.3.1 Models showing the steric hinderance between different lesions (colored yellow and turquoise)and DNA. Steric hinderance causes double helix destabilization and refers to the degree of crowding between different atoms.

2.4 Biomass Research: Cellulase Enzyme Structure-Function Relationships (Gregg T. Beckham, National Renewable Energy Laboratory)

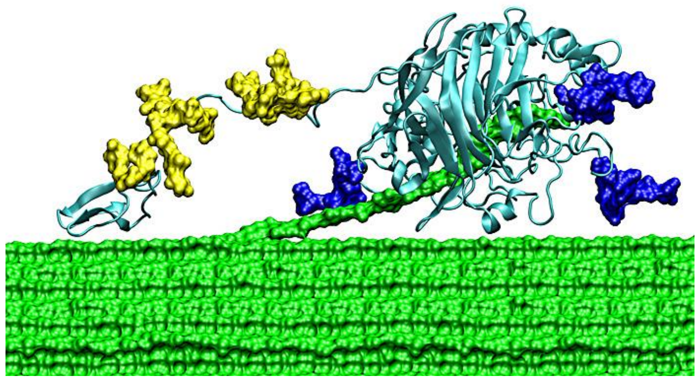


Figure 2.4.1 The Family 7 cellobiohydrolase from *T. reesei.*

Plant cell wall polysaccharides such as cellulose and hemicellulose offer a vast renewable resource for the sustainable production of transportation biofuels and commodity chemicals through industrial processing, but plants have evolved these structural polymers as natural defense mechanisms to resist infection and degradation. As plants represent a vast source of energy for organisms from all kingdoms of life on Earth, many biological paradigms have evolved to deconstruct these polymers to sugars. These natural biological degradation strategies offer an obvious starting point for harnessing their capability in an industrial context to produce biofuels. To that end, Beckham and colleagues use a variety of computational methods at varying resolution, from quantum mechanical calculations to large, atomistic molecular dynamics simulations, up to coarse-grained resolution models to understand the mechanisms that Nature employs to break down cellulose and hemicellulose into their component sugars. Understanding the various steps required for biomass degradation at different length and time scales requires a broad range of computer architectures, which makes XSEDE resources ideal for this type of work. In particular, Beckham and colleagues conduct quantum mechanical calculations to examine the electronic structure of plant cell wall carbohydrates and to understand enzymatic reactions to break polysaccharides down into the component sugars. These types of calculations require significant memory, which are ideal for PSC and SDSC resources. Classical molecular dynamics simulations of enzymes and large crystalline substrates, as would be found when an enzyme is degrading cellulose in the plant cell wall, require computer architectures with fast interconnects for parallelization and fast compute nodes. These types of simulations are ideal for resources at NICS and TACC. Overall, the variety of XSEDE resources available is enabling the group’s multiple types of projects to occur simultaneously and efficiently, with the overall aim of understanding and engineering enzymes for more efficient conversion of lignocellulosic biomass to renewable biofuels. To date, the NREL group has predicted new roles for glycosylation on cellulase enzymes, elucidated new roles for the individual sub-domains in cellulases, and revealed new understanding about inhibition of enzymes by their disaccharide product, cellobiose. More recently, they have used quantum mechanical calculations and hybrid quantum mechanical/molecular mechanics methods to elucidate various aspects of cellulose hydrolysis.

2.5 Novel Studies of Gene Regulation in Brain Development May Mean New Treatment of Mental Disorders

A research team at UC San Diego and the Institut Pasteur, Paris has come up with a novel way to describe a time-dependent brain development based on coherent–gene-groups (CGGs) and transcription-factors (TFs) hierarchy. The findings could lead to new drug designs for mental illnesses such as autism-spectrum disorders (ASD) and schizophrenia.

In the paper, published November 22 as an online-first publication in the journal *Genes, Brain and Behavior*, the researchers identified a hierarchical tree of CGG–TF networks that determine the patterns of genes expressed during brain development and found that some "master transcription factors" at the top level of the hierarchy regulated the expression of a significant number of gene groups.

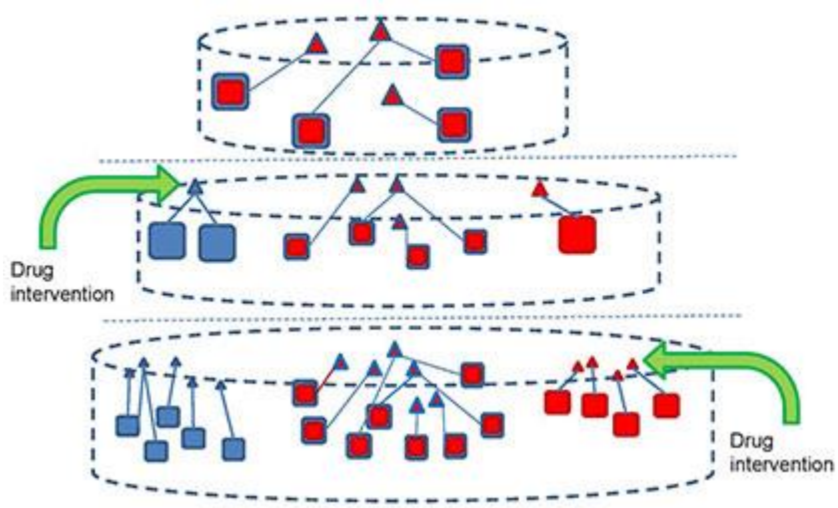


Figure 2.5.1 Diagram showing the hierarchy of TFs and CGGs networks and the novel strategy of drug design based on hierarchical gene–TF network analysis. The blue squares are schizophrenia-related; the red squares are autism-related CGGs and TFs. Some CGGs and TFs are common for both disorders, while some are unique for each disorder. The different levels represent genes responsible for different parts of development. Drugs can be administered at different levels of hierarchy and delivered either to a set of possible targets or the selected CGG. *Courtesy of Igor Tsigelny, SDSC/UC San Diego*

Instead of taking the approach that a single gene creates a single response, researchers used contemporary methods of data analysis and SDSC's Gordon supercomputer to identify CGGs responsible for brain development, which can be affected for treatment of mental disorders. The relevant drugs must be delivered at very specific times of development to be effective.

"We have proposed a novel, though still hypothetical, strategy of drug design based on this hierarchical network of TFs that could pave the way for a new category of pharmacological agents that could be used to block a pathway at a critical time during brain development as an effective way to treat and even prevent mental disorders such as ASD and schizophrenia," said lead author Igor Tsigelny, a research scientist with SDSC, the UC San Diego Moores Cancer Center and the university's Department of Neurosciences. "On a broader scale, these findings have the potential to change the paradigm of drug design."

Using samples taken from three different regions of the brains of rats, the researchers used Gordon and SDSC's BiologicalNetworks server to conduct numerous levels of analysis, starting with processing of microarray data and SOM (self-organizing maps) clustering, before determining which gene zones were associated with significant developmental changes and brain disorders. Researchers then conducted analyses of stages of development and quick comparisons between rat and human brain development, in addition to pathway analyses and functional and hierarchical network analyses. The team then analyzed specific gene–TF interactions, with a focus on neurological disorders, before investigating further directions for drug design based on analysis of the hierarchical networks.

3 XSEDE Project Office 1.1

3.1 Overview

The last quarter of the calendar year is always challenging due to the SCxy conference and holidays. We have become quite effective at scheduling around such events and continued to show solid productivity in the second quarter of Project Year 2 (PY2). Unfortunately, during this quarter our XSEDE External Relations Coordinator, Susan McKenna, moved on to another position. A search for her successor has begun.

The SC12 conference in Salt Lake City, Utah and the XSEDE exhibit along with the Annual Highlights book were major accomplishments for the project this quarter. The booth saw many attendees coming to find out more about XSEDE and was the nexus for many new connections with the community.

The development of the Component Registry—a joint effort of the Systems & Software Engineering, Architecture & Design Team and Software Development & Integration teams—made significant progress this quarter and we are on track to be able to easily track and report on status of key components throughout XSEDE processes, from the architectural stage, through development and integration, and on to production operation. This will provide much greater visibility an assessment of overall progress in satisfy the support of the Use Cases that encapsulate the needs of the researchers we support.

During the past quarter, the Architecture & Design team (A&D), in conjunction with the Systems & Software Engineering team and major stakeholders, has focused on developing a large number of Use Cases previously identified as priorities in the project. This has been an effort both to optimize the Use Case Development process and to allow a global prioritization of Use Cases once a large number have been documented. The intent is to reach a point where we can prioritize based on individual use cases and now on general areas as we have previously been pursuing this. This will allow us to deliver the highest value Use Cases sooner. The team has developed a weekly cadence for development of these Use Cases that is proving to be quite effective. This has facilitated more efficient design and reviews of the architectural components as part of the L3 decomposition.

After really coming together as an effective area, our Systems and Software Engineering (S&SE) effort has really begun to hit their stride this quarter. Many of their activities are now becoming more routine and manageable to the benefit of the project. S&SE has become more efficient in its ongoing efforts to identify and elicit new user needs and capabilities in order to improve and "grow" XSEDE. The development of Use Cases with the Architecture & Design Team and key stakeholders is something that S&SE staff have also gained a lot of experience with as our partners at the Software Engineering Institute phase out of this role. The XSEDE Digital Object Repository has begun to take shape again after our interruption in the process with the loss of our External Relations lead.

The Software Development and Integration (SD&I) has also been making great progress working to close out the raming 5 of the origin 100 activities planned as part of "*Increment 2*" and initiating 16 activities prioritized by the User Requirements and Prioiritization Working Group for "*Increment 3*." This was the first instance of fully utilizing our prioritization process to guide the activities of SD&I.

With our Sciforma project management software in and fully populated, our Project management and Reporting team has been able to use it to respond to report requests and to update the project schedule with new activities and progress. Additionally, we have made progress on assessing the use of the Baldrige in the context of the XSEDE project and how it can be used to drive improvement.

Our October 12, 2012 XAB teleconference had a focus on our Industry Relations Program. This discussion resulted in firm guidance about moving the area forward within the project and the development of a call for participation in an "XSEDE Industry Challege." A plan for this will be developed once a Level 3 manager is identified including risks and resource usage.

3.2 Project Management and Reporting 1.1.1

Prepared ECSS quarterly reports – information was requested for over 80 projects

Provided ECSS metrics to Dave Hart

Updated project schedule with new activities and progress

Worked outstanding Sciforma issues with Vendor

Refreshed Sciforma Test Environment with production data and reapplied new security/tokens settings

Worked with Level 2/3 WBS managers on PY3 planning and quarterly reporting

Created draft "call for interest" for Industry

Updated risk register

Worked on white paper to address the NSF review team's request to review XSEDE with appropriate use of the Baldrige criteria

3.3 Systems and Software Engineering 1.1.2

During the quarter ending 12/31/12, the Systems and Software Engineering Team has accomplished the following:

3.3.1 Gathering New User Needs and Capabilities

SSE continued its ongoing efforts to identify and elicit new user needs and capabilities in order to improve and "grow" XSEDE. SSE staff participated in the user facing project areas of XSEDE (ECSS, the NIP group in particular, User Engagement, and Campus Champions, etc.), joining in their regular conferences calls and email discussions to tease out new user needs and capabilities. We also review reports of meetings, conferences, surveys, and other user outreach events for similar information. The information collected is of a widely disparate nature, from simple requests and fixes to things that are much more complex and have architectural significance. We also participate in discussions about how best to get these capabilities and needs into the XSEDE "pipe" for processing by the appropriate group.

3.3.2 Use Case Development

The XSEDE Architecture and Design Group has identified several areas of strategic importance for the XSEDE architecture including: science gateways, data analytics, high performance computing, high throughput computing, scientific workflows and visualization. Appropriate Subject Matter Experts (SMEs) have been identified for each of these areas and asked to develop use cases for their subject area. Since developing use cases is a new concept for the SMEs, SSE staff have been working with these SMEs to help them generate effective use cases and quality attributes for each of these strategic activity areas. There are multiple uses cases under development for each of these activity areas.

3.3.3 XSEDE Component Registry

SSE and members of the XSEDE Architecture and Design, Software Development and Integration and Operations continued efforts to develop a registry of XSEDE components. The goal of this effort is to provide XSEDE management with a mechanism to easily track key components throughout XSEDE processes, from the architectural stage, through development and integration, and on to production operation. This will enable us to provide better tracking and reporting about the status of new capabilities that we have added to help XSEDE evolve and grow in response to changing user needs.

3.3.4 XSEDE Digital Object Repository

The XSEDE Digital Object Repository will be used to preserve all the key documents and digital objects of the XSEDE project via the University of Illinois IDEALS archival system. During this quarter we developed an appropriate document naming scheme and organizational structure for the XSEDE document collection and identified a set of key foundation documents that will be the first documents stored in the archive.

3.4 Architecture and Design 1.1.3

During the second quarter of program year 2 (PY2) the A&D team focused on the collection, process of tracking and reviewing the rapidly growing number of XSEDE use cases. Significant efforts were made by David Lifka and Altaf Hossain to engage the XSEDE architectural area leads, identify new architecture use case areas, and to train and assist area leads in the development of use case documentation including proper quality attribute scenarios.

By engaging all the various area leads (over 25 active participants now) and encouraging them to develop use cases while XSEDE still had access to Felix Bachmann for guidance and support, the A&D team was able to quickly identify inefficiencies and bottlenecks in the A&D processes as part of the overall XSEDE software engineering process. Our weekly Thursday team calls have become extremely productive, focused on the architects reviewing use cases that have been prepared by the area leads that have been reviewed, refined and approved by Altaf Hossain. Altaf's expertise in use case and quality attribute scenario development has dramatically improved the quality of the use cases before the architects are asked to review them making team calls much more efficient. The XSEDE architects, the SD&I team led by JP Navarro and Felix Bachman had in depth meetings and discussions how best to effectively review and approve the rapidly growing volume of architecture and use case documentation. As a result processes, particularly use case and active design reviews, are continuing to become more efficient. Friday Architects calls have been focused on Active design reviews and prioritization of next use cases and L3 decompositions to focus on next.

3.4.1 Use Cases Creation

We now have over 50 use cases in various stages of development and review. As we reviewed some of the initial use cases from the Campus Bridging and Science Gateway areas it became evident that there were basic use cases that several of the areas needed such as "Submit a job", "Transfer a file", and "Authenticate". We have initially identified 10 of these canonical use cases. The architects will focus on documenting these and preparing the level 3 decompositions so that other area leads can simply refer to them or identify special features or requirements they have in addition to them. These canonical use cases will again improve documentation and review efficiency for the overall software engineering process.

We have also been approached by Shantenu Jha and Ole Weidner from Rutgers to create a new architectural area for Federation and Interoperation use cases.

Number of use cases by architectural area:

- Campus Bridging (7)
- Science Gateways (5)
- Computing
  - High Performance Computing (4)
  - High Throughput Computing (5)
  - Scientific Workflows (2)
- BIG Data
  - Data Analytics (5)
  - Data Movement, Storage, Backup & Archival (5)
  - Visualization (3)
- Connecting Instrumentation (1)
- Collaboration (1)
- Canonical (10)
- Federation and Interoperation (1)

3.4.2 Development of a Use Case Registry System

David Lifka (A&D), JP Navarro (SD&I), Victor Hazlewood (SYS-OPS), and Janet Brown (SSE) have continued the development of a "Use Case Registry" system. This registry system will allow our team members and XSEDE management to track any use case throughout the software engineering cycle. Susan Mehringer from Cornell with support from JP Navarro is currently developing our first version of this system with a goal of having all of the A&D processes incorporated and ready for team use at the completion of PY2. This web-based system will provide views for various stakeholder groups so that they can track progress on their use case submissions.

3.4.3 *Q2 Activities*

- **XSEDE Architecture Documentation**

  A new version of the XSEDE Architecture Level 3 Decomposition has been produced that has a main architecture document with separate use case documents that refer to it. These documents are scheduled to be made public quarterly and each section will clearly state the current review and acceptance status of each architectural component. This will allow us to have a public facing document that continually evolves over time.

- **Number of new use cases per area**

  Over 50 new use cases in various stages of development and review.

- **Number of use cases accepted in the A&D process**
  11 use case ready for architects to prepare level 3 decomposition.

- **Active Design Reviews**

  Currently reviewing the security component of the XWAVE and XUAS architectures.

- **Use Case Registry System Development**

  Development of system covering A&D Processes and review is underway.

3.4.4 *Q3 Planned Activities*

- **XSEDE Architecture Documentation**

  Updates including several canonical use cases with Level 3 decompositions and Campus Bridging and Science Gateway use cases that build on them.

- **New use cases developed and accepted in the A&D process**

  Continued efforts to produce, refine and review new use cases and accept them into the A&D Process.

- **Active Design Reviews**

  Continue to focus improving the active design review process for efficiency and turnaround of important new capabilities.

- **Use Case Registry System Development**

  Will be ready for initial use by the XSEDE team by the end of PY2.

3.5 External Relations 1.1.4

3.5.1 *Accomplishments*

The XSEDE exhibit at the SC12 conference in Salt Lake City was a major achievement of the quarter. Preparation included updates to printed collateral such as the "What is XSEDE" one-pager, coordination of booth staffing, overseeing shipping of materials, and other logistics tasks. During the conference, XSEDE ER team members and other XSEDE staff continuously staffed the booth during exhibit hours, promoting the project to the conference's thousands of attendees.

The annual highlights book was completed (including coordination with design contractor and final proofreading) and shipped to Salt Lake City for distribution at SC12. Boxes of the highlights publication were distributed to the XSEDE sites represented at the conference and additional boxes were shipped by request following the event.

The team continues to compile and distribute two monthly newsletters, Inside XSEDE (for internal audiences) and What's New in XSEDE (for external audiences). This quarter new XSEDE staffer Liz Murray took over responsibility for the two newsletters.

Other ongoing efforts include: planning for XSEDE13, including participation in Key Leads and Logistics & Local Arrangements committees; regular updates to XSEDE website, as well as to the XSEDE13 site and other micro-sites;

3.5.2 Media Hits

Approximately 30 news items were published on XSEDE-related topics. An Excel file containing specific media hits has been submitted for inclusion in the Appendix.

3.5.3 Challenges

The XSEDE ER coordinator position is currently vacant after the departure of Susan McKenna in the fourth quarter. A search for her successor has begun.

3.6 Industry Relations 1.1.5

During the October 12th XAB teleconference call, we had a lengthly discussion regarding the Industry Relations Program. Topics discussed included what it would take to restart the effort in Industry Relations. It was determined that having a Level 3 manager would be very helpful. The XAB wanted to be sure that the expertise and resources would be available to achieve success. Another topic discussed was how to get Industry interested in participating in the Industry Relations Program. A discussion about working on classes of primary problems that span industry would be a good place to start. A suggestion was made to have a Call of Interest to Industry. The "Call of Interest" was drafted and is being reviewed. A Plan will be developed once a Level 3 manager is identified including risks and resource usage.

3.7 Software Development and Integration 1.1.6

As previously reported, Software Development and Integration (SD&I) "*Increment 2*" activities began in February 2012 with our first *semi-annual* planning activity. From over 100 identified activities 16 were prioritized and became SD&I's primary focus between PY1 Q4 and PY2 Q1 (April 2012 thru September 2012). This past quarter we continued to make progress on the 5 remaining incomplete increment 2 activities, most notably: testing an improved UNICORE 6 Execution Management Services (EMS) and Genesis II Global Federated File-System (GFFS), testing GridFTP support in UNICORE 6, and testing an upgrade to SP GridFTP software.

Also previously reported, SD&I "*Increment 3*" priorities were established in September 2012 by a User Requirements Evaluation and Prioritization (UREP) team. This was the first time that a team with User Advisory Committee (UAC) and XSEDE senior management representatives directly set SD&I priorities. Based on UREP established priorities, this quarter SD&I identified over 30 candidate development activities and selected a subset of those for effort between PY2 Q2 and PY2 Q3 (October 2012 thru March 2013). Specific increment 3 accomplishments this quarter include:

- Designing an improved *XSEDE accepted certificate authority configuration file* installer and distribution mechanisms to improve grid service and software configuration (SDIACT-003).
- Designing a command-line single sign-on hub/server that will enable users to login via ssh to an XSEDE wide login server, and then login to any other XSEDE login node without having to re-authenticate (SDIACT-070).

- Preparing a Globus Connect Multi-User installer that will significantly simplify Campus deployment and operation of GridFTP servers for moving data to/from their resource using Globus Online (SDIACT-108).
- Developing a System-wide Genesis II installer that will make it easier to install and use Genesis II software on SP resources (SDIACT-099).
- Significant progress re-designing and streamlining SD&I activity management wiki workspaces, documentation, deliverable templates, and assessing the JIRA tool to facilitate activity management (SDIACT-103, SDIACT-121).
- Conducting a design and security review of an improved xdusage utility enabling users to view allocation usage information from SP login nodes (SDIACT-102).
- Launching an effort to prepare a Globus Online Transfer REST API so that software developers can use Globus Online Transfer from their software (SDIACT-106).
- Prepared two plans for senior management that: 1) details the Campus Bridging pilot activities and schedule, and 2) detail Campus Bridging *production* activities and schedule.

4 XSEDE Operations 1.2

4.1 Overview

The Operations group consists of ~30 FTEs and is responsible for implementing, delivering, maintaining, and evolving an integrated cyberinfrastructure capability of unprecedented scale that incorporates a wide range of digital capabilities to support the national scientific and engineering research effort. The Operations group follows the XSEDE project management methodologies detailed in the Project Execution Plan by allocating and coordinating staff in accordance with the XSEDE work breakdown structure (WBS), scheduling tasks in the XSEDE project schedule, and identifying and reviewing risk on an ongoing basis. Operations staff is subdivided into six teams based on the WBS:

1.2.1 Cybersecurity
1.2.2 Data Services
1.2.3 XSEDEnet (Networking)
1.2.4 Software Testing and Deployment
1.2.5 Accounting and Accounts Management
1.2.6 Systems Operational Support

This quarter the Operations team's activities included the purchase of One Time Password tokens to begin testing the XSEDE OTP service. Work began to implement storage allocations within the XSEDE allocations process, POPS, and service provider accounting systems. Detailed configurations and pricing for the distributed hardware that will host the XSEDE-wide file system were finalized. Internet2 was selected to provide connectivity for the XSEDE federation. Despite several planned and unplanned outages during Q2 of PY2 the SysOps team maintained high overall uptime, which ensured data integrity and availability. During the Q2 of PY2 the XSEDE Operations Center (XOC) fielded 2,098 tickets and closed 2,021 tickets.

4.2 Cybersecurity 1.2.1

The Security Operations team's focus is the availability, integrity, and security of XSEDE related information, data, and services. No vulnerabilities were identified within this quarter that required XSEDE-wide notification, and there were no known compromised user accounts and no security issues with XSEDE resources.

CA and Kerberos Administration
The responsibility for the XSEDE Kerberos realm has been moved from XSEDE centralized services to Security Operations. This was largely due to the fact that the XSEDE Kerberos realm is administered at NCSA and is tightly connected to a separate NCSA realm.

XUP credential exposure in Java applet
A JAR file was discovered that is used by the portal and contains valid credentials that could allow an attacker to access the XSEDE Central DB. While the credential only allowed read access, XSEDE user information (email, names, address) could have been collected. Security Operations contacted User Information and Interfaces who removed the JAR file and pushed out an update to the portal to resolve the issue. The credentials that were used have been invalidated and/or changed. A suggestion to developing security training-material for XSEDE technical staff resulted and an activity will be added to the XSEDE schedule for Security Operations.

GX-Map cadesc support with CA Tarball updates
A 'beta' version of the GX-Map software that adds support for DER formatted CRLs and has a new tarball of the CAs and the CAdesc files ready to be tested.

One Time Password (OTP)
A quantity of 250 RSA tokens have been ordered to begin testing of the One Time Password system that will be deployed for XSEDE staff. The OTP service is being coordinated with SD&I for evaluation and configuration.

Checklist for Departing Security Staff
The staff exit checklist/process was recently updated to include recommendations and comments from the group. Security Operations will review the system characterization section of the Risk Assessment to see if there are other services or assets that should be included in the checklist.

Host CA Update and InCommon CA News
InCommon has submitted their membership and/or CP/CPS to Derek Simmel, chair of the TAGPMA. The initial review of the InCommon CP/CPS is nearing completion. Once the InCommon CA is approved by the TAGPMA, XSEDE will start to leverage this for all of our Host CA certificate needs.

Risk Assessment Completed/Implementing Recommendations
With the completion of the risk assessment, Security Operations plans on implementing the high priority controls as recommended on the Control Recommendations Page. The first area of focus is policy: https://www.xsede.org/web/staff/staff-wiki/-/wiki/Main/XSEDE+Security+policies.

Qualys Vulnerability Scanning
The one-year evaluation of the Qualys vulnerability scanning tool is ending and Security Operations will place an order for a license to cover the most critical XSEDE hosts.

MyProxy CA Downtime Reponse Report
The MyProxy service experienced downtime on November 6th due to a hard drive failure. The fail-over took longer than expected prompting NCSA to review the continuity plan to avoid similar outages in the future. Procedures for failover have now been documented and the hardware that failed has been replaced.

Security enhancement rollouts
Changes were made to the XSEDE Approved Certificate Authorities: On 11/1/2012 the expired UK EScience CA certs and files 367b75c3.* were removed and filenames and symlinks were corrected.

4.3 Data Services 1.2.2

The Data Services group facilitates data movement/management for the XSEDE community by maintaining and evolving data services and resources. Data Services activities for this quarter included maintaining the existing operational infrastructure, such as GridFTP servers and archive resources, improving documentation for data resources in XSEDE, and preparing for upcoming software deployments and accounting changes.

The XSEDE-Wide File System (XWFS) process continued with detailed planning of hardware deployments, software configuration, and costs across all participating sites. Data Services team members from TACC, SDSC, NICS, PSC, and NCSA were engaged in this process and helped both to refine deployment plans and to prepare local infrastructure for installation of the XSEDE Wide File System.

Several SD&I components effecting Data Services remain in preparation for deployment, including updates to GridFTP, Globus Online, and the Global Federated File System. Operations staff continued to participate in testing and operational readiness reviews for all such components. In addition, Data Services became more engaged in development of use cases for Architecture and Design, developing drafts of three use cases and planning for several additional use cases in the area of data transfer, management, and archival.

The Albedo wide-area file system has now been retired, and data migration operations to move users and user data to appropriate alternative resources were completed during the quarter. PSC staff led the data migration effort and staff from SDSC, TACC, NICS, and Indiana was involved in completing the migration and shutdown efforts for Albedo hardware.

Additional efforts were initiated to improve data transfer metrics, accounting for individual data resource performance, network interactions, and issues of resource contention. Efforts in the quarter were focused on planning and work will continue in cooperation with SD&I and other areas to implement specific features and services in support of improved monitoring of and accounting for data transfer performance.

4.4 XSEDEnet 1.2.3

The Networking team's primary focus is monitoring, maintaining, and improving XSEDEnet. Ongoing discussions were held with Internet2 to determine how they could meet the need for XSEDE Service Provider connectivity. Contract negotiations are the next step.

Figure 11, Appendix E shows traffic utilization of the Chicago-Denver link for 4Q2012. Figure 12, Appendix E shows link utilization as a percentage. Traffic offered load into XSEDEnet links for 4Q2012 is shown in Figure 13, Appendix E.

The following table summarizes network outages for the quarter by site.

Map	Device	Up	Down	Uptime	Downtime	Times Down
XSEDE	FutureGrid	99.88%	0.12%	91 days 21:2	2:33:16	5
XSEDE	IU	99.89%	0.11%	91 days 21:3	2:27:29	4
XSEDE	NCSA	94.61%	5.39%	87 days 1:3:4	4 days 22:56	206
XSEDE	NLR-CHIC	100.00%	0.00%	92 days 0:0:0	0:00:00	0
XSEDE	NLR-DENV	100.00%	0.00%	92 days 0:0:0	0:00:00	0
XSEDE	PURDUE	99.89%	0.11%	91 days 21:3	2:29:24	4
XSEDE	SCSC	99.56%	0.44%	91 days 14:2	9:39:24	29
XSEDE	UCAR	99.75%	0.25%	91 days 18:2	5:34:15	15
XSEDE	PSC	99.92%	0.08%	91 days 22:1	1:42:30	6
XSEDE	TACC	94.59%	5.41%	87 days 0:35	4 days 23:24	211
XSEDE	NICS	94.28%	5.72%	86 days 17:4	5 days 6:17:4	161

4.5 Software Testing and Deployment 1.2.4

Operations Software Testing and Deployment (ST&D) identifies resources for software testing, conducts acceptance testing and operational readiness reviews of software, and aids the deployment of software at service providers. The Software Deployment and Testing (ST&D) group completed operational readiness reviews (ORRs) for three Configuration Items (CIs) this

quarter:

* Globus Online Update (SDIACT-50 and SDIACT-100)

* Basic Execution Management Services (EMS) (SDIACT-97)

* GridFTP Update (SDIACT-31)

Acceptance testing for the Globus Online Update was completed during this quarter, and a production deployment addressing the security concerns from previous reviews was initiated. Acceptance testing for Basic EMS was also begun this quarter, and is expected to be completed early next quarter. Acceptance testing for the GridFTP Update will begin in the next quarter.

The GFFS beta deployment continued to be a major area of effort in the ST&D group this quarter. Test services for the beta were deployed at NICS, PSC, and TACC, and staff testing at those sites was completed. Alternate packaging methods for the Genesis II software were also investigated. The campus bridging pilot sites are expected to begin their testing next quarter.

	PY1 Q1	PY1 Q2	PY1 Q3	PY1 Q4	PY2 Q1	PY2 Q2
CI Readiness Reviews Completed	0	0	2	1	0	3
CI Acceptance Tests Performed	0	0	2	1	0	1
CIs Accepted for Beta	0	0	0	1	1	0
CIs Accepted for Production	0	0	0	0	0	1
CIs Deployed for Beta	0	0	0	0	0	1
CIs Deployed for Production	0	0	0	0	0	1

4.6 Accounting and Account Management 1.2.5

The Accounting and Account Management (A&AM) group maintains and improves the interfaces, databases, and data transfer mechanisms for XSEDE-wide accounting of resource allocation and usage. In this quarter, the work in the Partnerships Online Proposal System (POPS) to support variable length allocations was completed, tested and implemented. This functionality enables allocations to be any length, rather than the traditional one-year, and will be used for educational and training allocations, as well as for FutureGrid allocations.

Accounting for TACC's Stampede system was implemented in POPS and the XSEDE Central Database (XDCDB). Work also began on making the transfers from the TACC Ranger system to Stampede, and will continue into the third quarter of this year.

Planning began on a formalized implementation of Storage Allocations in POPS and the XDCDB. While storage-based allocations have been awarded in the past, there were no special rules in place to reflect the unique nature of these types of allocations. Some of the capabilities that have defined to date include: stand-alone storage allocations; enforced limits; default allocations; etc. Implementation has already begun in POPS on the features that have already been agreed upon.

A team has been formed to design and develop the new "POPS 2.0" system, which will be a complete re-write of the POPS system, using the XDCDB PostgreSQL platform, and integrated more closely within the XSEDE User Portal. The targeted completion date for this re-write is second quarter of program year three.

4.7 Systems Operational Support 1.2.6

The Systems Operational Support (SysOps) group is responsible for operating the XSEDE Operation Center and providing system administration for the ever-evolving set of XSEDE centralized services. Significant progress was made in the following WBS tasks in Q2 of PY2: 1.2.6.10 and 1.2.6.12. Tasks worth noting include cross group collaboration with User Engagement to finalize RT deployment schedule, weekly operations RT team status calls, a complete refresh of the central Nagios monitoring instance, and continued support for the Genesis II Campus Bridging Pilot program. Even though there were several planned and unplanned outages during Q2 of PY2 the SysOps team maintained high overall uptime, which ensured data integrity and availability. By leveraging failover resources, where appropriate, user-facing downtime was greatly minimized. As such, no central service experienced any less than 91.17% uptime for Q2 of PY2. In this instance we uncovered a missing step in our notification procedures, as the Karnak application administrator was unaware that the service was unavailable for that long. With this exception in mind, none of the other central services experienced less than 99.64% uptime during the quarter.

4.7.1 XSEDE Operations Center

During the Q2 of PY2 the XSEDE Operations Center (XOC) fielded 2,098 tickets and closed 2,021 tickets. Among these 1,872 were submitted via email to help@xsede.org, 18 were submitted via the XSEDE User Portal, and 208 were submitted via phone to the XOC. There were 72 tickets closed within 2 business days, which equates to 35% for the reporting period. There were a total of 1727 tickets responded to within 24 hours, which equates to 82% for the reporting period. Table 16, Appendix E shows the ticket breakdown (opened/closed) for each major resolution center. Figure 16 in Appendix E shows tickets broken into the 7 distinct problem categories with significant representation.

4.7.2 Central Services

There were several outages both planned and unplanned that affected various central services during Q2 of PY2. Many of these outages were the result of individual servers or sites experiencing unexpected technical difficulties or routine maintenance. Outages varied between site-specific power events, networking interruptions, system failures, planned activities, and user initiated interruptions.

The following table describes each service that experienced an outage, the corresponding downtime/uptime, the nature of the outage (e.g. Planned or Unplanned), and the total number of hours down:

Service	Percentage of Uptime	Planned Outage(s)	Unplanned Outage(s)	Total Outage(s)
Certificate Authority	**99.73%**		6 hours	**6 hours**
INCA Backup	**99.91%**		2 hours	**2 hours**
Karnak	**91.17%**		195 hours	**195 hours**
RDR	**99.64%**		8 hours	**8 hours**

XDCDB	**99.89%**	.06 hours	2.25 hours	**2.33 hours**
XDCDB Backup	**99.64%**		8 hours	**8 hours**
XUP Backup	**99.91%**		2 hours	**2 hours**

The remaining services did not experience an outage during the reporting period.

4.7.3 INCA

At the time of this report, the Inca deployment was executing 1063 tests for XSEDE software and services. Of these, 120 of these tests were running for six central XSEDE services: Inca, Information Services, Karnak, MyProxy, User Portal, and XDCDB. The table below shows the definition of an outage for each service and the uptime percentages as detected by Inca. All services fall within acceptable limits of their high availability service definition.

Service	Definition of outage	Uptime (Details of outages)
Inca	Inca status pages are unavailable or not able to fetch data from the database (i.e., test details page fails to load). Tests every 5 mins.	**99.71%** (One outage for 6.5 hours of downtime)
Information Services	Information Web pages are unavailable. Tests every 15 mins.	**99.76%** (Two outages for a total of 5.3 hours of downtime)
Karnak	Karnak front page fails to load. Tests every 30 mins.	**91.17%** (Two outages for a total of 195 hours of downtime)
MyProxy	MyProxy server does not respond to credential query check. Tests every hour.	**100%** (No outages detected)
User Portal	Portal front home page fails to load correctly. Tests every 30 mins.	**100%** (No outages detected)
XDCDB	Connection to database refused or slow (using check_postgres.pl script). Tests every 5 mins.	**100%** (No outages detected. Note that both Inca and the XDCDB were down simultaneously)

4.7.4 Syslog Monitoring Project

The Cornell Center for Advanced Computing (CAC) has partnered with XSEDE sites including the Texas Advanced Computing Center (TACC) and the Pittsburgh Supercomputing Center (PSC) in order to provide a novel approach to systems administration and monitoring. Most recently, CAC staff began collaborating with PSC by obtaining a data sample from them, processing this sample into our system, and began initial analysis. In addition, CAC staff have authored a technical paper on work to date. This paper will be completed early in Q1 2013. Finally, CAC staff updated the log analysis and monitoring system from SQLstream 3.0beta to

SQLstream 3.0, which now runs on a Red Cloud computing node for on-demand analysis as the collaboration with PSC continues to expand.

4.7.5 Globus

During the reporting period, there were 14 million files transferred to and 18 million files transferred from XSEDE endpoints using Globus Online (GO). In total GO facilitated transfers of 559 TBs to and 453 TBs from XSEDE endpoints. There are currently 217 distinct GO XSEDE users. Diving deeper we know that of the total files transferred 2 million were transferred from Globus Connect (GC) to an XSEDE endpoint and 5 million files were transferred from an XSEDE endpoint to GC. In total 37 TBs of data were transferred from GC to an XSEDE endpoint while 23 TBs were transferred from an XSEDE endpoint to GC. Of the previously mentioned distinct XSEDE GO users, 124 of them are distinct GC users. This data does not include stats from automated performance testing.

In total, there were 23 tickets opened for the GO team. The tickets can be lumped into the following categories: user education, endpoint operational issue, bug fix, feature request, and user action required notification. The table below shows the number of tickets that fit within each distinct category.

Category	Number of Tickets	Explanation and Details
User Education	4	Information provided to resolve the problem.
Endpoint Operational Issue	11	Problems using a specific endpoint.
Bug Fix	5	A problem occurred that warrants a change/fix to the GO software/system.
Feature Request	3	GO lacking in some way and an improvement/new feature is identified.
User Action Required Notification	0	Unsolicited email sent to user(s) for a problem that they should be aware of.

5 User Services 1.3

5.1 Overview

The XSEDE User Services operational activities continued to provide high quality user support for a diverse national user community. The quarterly allocations committee meeting awarded allocations totaling 427M cycle-hours out of 439M available hours (on requests of 1.1B), including awards on the new Stampede system. There were 15 training activities, including the first multi-site course on OpenACC, reaching over 8000 attendees (in person, and online), with another 19 already scheduled for Q1CY2013. User support tickets continued to be resolved and mined for patterns, revealing that storage systems, data transfers, and availability of specific software packages are the current top issues documented in user tickets. The second user survey was initiated, incorporating lessons learned from the initial survey. User documentation continued to expand with new documents covering Stampede and the BigJobs community code. The XUP continued to improve existing features such as the change password procedure, and add new capabilities including *add user* (to an allocation).

In short, XSEDE's operational user support activities are operating smoothly and effectively. In addition, several 'project' activities are making progress and should complete in CY2013. The new ticket system is being deployed, the training certification process is advancing, a new mobile device web interface is being developed, and the storage allocations process should be implemented before the end of project year 2. Details on all of these activities and others are given below.

5.2 Training 1.3.1

The XSEDE training efforts continued this quarter at a pace that will exceed our annual goals. Training reached more than 8,000 people via online, webcast, and in person methods. Fifteen scheduled events took place, including a large multi-site simulcast course on OpenACC. These events had more than 850 registrants. Demand for both beginner and advanced training continues to grow. In online training, about 700 users completed courses via CI-Tutor, and 7,000 more visited the virtual workshop site (more than 1,500 of these were repeat visitors).

The first quarter of the calendar year will be an exceptionally busy one, with Stampede training ramping up as well as a number of other activities. Nineteen training events are already scheduled for the first quarter, with more on the way. Planned outreach to MSI campuses continues with a heavily subscribed visit to UTEP, as well as events in planning at FIU and UMBC.

Conversations continue on coordination with the VSCSE (Virtual School for Computation Science and Engineering) and VSCSE training event registration will be managed by the XSEDE User portal this summer. The plan for training certificates was presented for review at the December quarterly, and implementation is proceeding on schedule.

Overall, in both delivery and in course development, XSEDE remains on track to deliver on the milestones for this year.

5.3 User Information & Interfaces 1.3.2

Both the XSEDE web site and XSEDE User Portal (XUP) released new features and met deliverables for this quarter. The XSEDE web site continued to expand and improve the online content by adding and updating new user guides including the Stampede User Guide and the BigJobs community code user guide. To assist PIs with the proposal writing process a new set of successful sample allocation proposals were collected and posted. Also the UII team integrated additional services and test bed categories into the resources listings – services now include

Globus Online and FutureGrid has been added as a test bed category. Integration of FutureGrid into the XSEDE documentation was accomplished where appropriate such as the resources page, allocations, and more. Efforts this quarter also included collaborating with Campus Champions to create a dynamic campus champions directory. The directory displays a photograph and basic profile information of all the campus champions.

This quarter also included new features in the XSEDE user portal and improvements to the *add user* feature. The *add user* process was integrated into the POPS Sybase directory to facilitate faster request processing. Now add requests are processed within 24 hours, enabling users to begin working on a project much faster. Also, the publications feature was expanded to improve the user input interface and more effectively handle duplicates. XSEDE now has entries for over 275 publications that have been submitted via this feature. Backend improvements were made to both the password reset and change password features to more effectively integrate them into the Liferay environment. Finally, during the reporting period there were over 37K file transfers accounting for over 10TB of data transferred via the portal file transfer service.

The Knowledgebase (KB) team expanded and improved KB articles by adding 36 new KB items and updating existing articles to insure accuracy. There are now a total of 573 documents in the KB and there have been over 187K document retrievals.

The usage of both the web site and user portal continues to increase with over 2.2 million hits on the web site and over 1.5 million on the user portal within the reporting period. Furthermore, over four thousand XSEDE users logged in to the user portal and 71% of the 2,225 users running jobs on XSEDE are logging in to the user portal.

5.4 User Engagement 1.3.3

XSEDE User Engagement is organized as two working teams: Feedback and Consulting. The Feedback team focuses on proactive support, while the Consulting team focuses on reactive support.

Feedback

The Feedback team completed all required feedback activities and required reporting for the quarter.

The Feedback team conducted a focus group entitled “Cloud Services” that explored computation, storage, and applications in cloud-like environments and a focus group entitled “XSEDE Survey Process” that explored possible approaches for effectively surveying users. Reports documenting the events are available on the XSEDE Staff Wiki. The team also conducted a BoF entitled “XSEDE User Meeting” at SC12. The BoF solicited feedback on a variety of XSEDE services such as training, allocations, consulting, and ECSS. A report documenting the event is posted on the XSEDE Staff Wiki for reference.

The Feedback team completed data mining on the tickets submitted to help@xsede.org during the previous quarter. As in previous quarters, the majority of tickets were related to routine operational issues. Aside from routine operational issues, the most common issues across XSEDE were related to data transfer, storage facilities, and specific software packages (such as Gaussian, Matlab, NAMD, VASP, etc…). A report documenting the results of the quarterly data mining activities is posted on the XSEDE Staff Wiki for reference. The data mining team also supplemented the report with a recommendation that XSEDE provide web-based training and documentation on data transfer methods within XSEDE and their recommended usage, along with an overview of where different types of data should be stored at various sites. The team also recommends training or quick-start guides for some of the major software packages within XSEDE.

The Feedback team formalized and implemented an on-going interview program to directly collect feedback from users concerning topics of specific interest to XSEDE. The initial round of interviews asked a selected set of Campus Champions about topics such as satisfaction, usability, access methods, documentation, consulting, data transfer, and the mobile XUP. A report documenting the initial round of surveys will be posted to the XSEDE Staff Wiki when it is available. Reports on future interview activities will be posted prior to the submission of the quarterly report for the quarter in which they are conducted.

As part of the integration of the Technology Investigation Service (TIS) with XSEDE, the TIS user advocate team merged with the Feedback team, and the combined team assumed the responsibilities to report feedback items pertaining to technology needs to the TIS and Systems Engineering teams and to gather technology needs from user interactions in ECSS and TEOS. This quarter, their activities included a report to TIS about salient items from the 2012 User Survey and a report about the findings of the workshop "Extending High-Performance Computing Beyond its Traditional User Communities," which was organized by ECSS on October 8, 2012, in conjunction with the 8th IEEE International Conference on eScience in Chicago.

Finally, the Feedback team formulated a new plan for conducting surveys within XSEDE and began work on the PY2 Annual User Survey. The new plan calls for a short, general satisfaction survey to be conducted annually. The annual survey will be supplemented with targeted surveys on specific services and activities. Polling and micro surveys will be used to support feedback campaigns about very specific topics of interest to XSEDE.

Consulting

The Consulting team conducted all required consulting activities for the quarter and made significant progress towards the milestones associated with the deployment and release of the new XSEDE ticket system. A detailed project plan for the deployment of and transition to the new ticket system is posted on the XSEDE Staff Wiki for reference. Deployment and training are expected to occur in PY2Q3, and transition to the new system for new tickets is expected in April of 2013. Decommissioning of the old system will commence once any open tickets in the old system are closed or migrated. Finally, a cost-risk-benefits analysis for the proposed XSEDE CRM is underway.

5.5 Allocations 1.3.4

This objective encompasses the allocations process, both for Startup, Education and Campus Champion allocations as well as the merit-review XRAC Research request process, the POPS system for request handling and management, mechanisms by which allocation PIs manage allocations through transfers, extensions and so on, and interfaces by which allocation PIs manage the users who are authorized to use their allocations. Operationally, this objective includes the XRAC review process, the Startup allocations review and decision process, and the maintenance and operations of the POPS system.

The table below shows the overall allocations management activity handled by POPS and the allocations staff for the reporting period. Note that for Transfers, the table shows only the positive side of the transaction to show the total transfer level; there is a corresponding negative amount, adjusted for resource exchange rates.

POPS Requests and Awards

	Research				Startup				Education				Campus Champions			
	# Req	SUs Req	# Awd	SUs Awd	# Req	SUs Req	# Awd	SUs Awd	# Req	SUs Req	# Awd	SUs Awd	# Req	SUs Req	# Awd	SUs Awd
New	73	227,633,708	64	85,902,706	130	21,152,223	101	11,749,047	6	630,210	5	480,000	8	7,478,047	7	4,449,005
Prog. Report	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Renewal	115	807,600,507	105	341,830,627	12	1,348,526	8	810,014	7	2,221,012	7	2,210,000	15	11,415,015	15	7,001,009
Advance	36	14,671,446	32	10,331,000	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Justification	8	15,595,500	1	3,100,000	0	0	0	0	0	0	0	0	0	0	0	0
Supplemental	28	34,547,494	8	4,071,000	11	2,280,015	9	905,000	5	264,000	5	254,000	9	605,000	6	425,000
Transfer	88	40,805,108	82	24,039,162	34	2,115,824	31	1,679,017	1	1,800	0	0	0	0	0	0
Extension	56	n/a	47	n/a	32	n/a	31	n/a	4	n/a	4	n/a	0	n/a	1	n/a

The December quarterly allocations meeting, XRAC, was planned and held in Orlando, FL. The next two XRAC meetings have been scheduled for Las Vegas, NV. in March 2013 and Indianapolis, IN. in June 2013.

Requests totaling 1.1B SUs were requested at the December 2013 XRAC meeting. Recommendations totaled 585M SUs with 439M SUs available. Many moves along with some cuts as much as 30% were needed to bring recommended awards in line with the individual resource available limits. However, the XSEDE Allocations staff and XSEDE site representatives are faced with a difficult situation of continued requests for supplements, transfers, and startups but no significant pool of SUs to satisfy the user community requests!

The XSEDE Allocations staff received 399 tickets within the reporting period. Most, if not all, were addressed and a high rate of user satisfaction achieved.

Lastly, XSEDE Allocations staff along with the XSEDE Operations/accounting group, led by Steve Quinn, are working on improving reporting of not only PI awards to their respective program officer but also to the entire XSEDE community via quarterly award announcements in conjunction with the XSEDE ER team.

6 ECSS – Projects 1.4

6.1 Overview

The Extended Collaborative Support Service (ECSS) pairs members of the XSEDE user community with expert ECSS staff members for an extended period to work together to solve challenging science and engineering problems through the application of cyberinfrastructure. In depth staff support, lasting weeks to up to a year in length can be requested at any time through the XSEDE allocations process. Expertise is available in a wide range of areas, from performance analysis and petascale optimization to the development of community gateways and work and data flow systems. ECSS staff members also participate in reviewing adaptive proposals associated with XRAC meetings.

In response to a User Survey finding that seemed to indicate that only 28% of users were aware of ECSS, we have begun working with External relations to publicize ECSS more widely. In a related matter, following up a suggestion of the User Advisory Committee, we are working with ER and User Services to allow users to post their own brief write-ups of achievements which XSEDE has enabled. This will include how ECSS has helped them achieve their scientific goals.

We followed up with Allocations to be informed of any supplements and time extensions on computing awards which change the end date of a project. We had been unaware that some projects had been extended, and expected continued ECSS support while our records showed that the project had ended.

ECSS efforts are divided into two parts, one designated as Projects, headed by Ralph Roskies; the other, designated as Communities, headed by Nancy Wilkins-Diehr. These groups have very close interactions, with common Project Management support. All told, ECSS consists of 37 FTEs, spread over ~80 people at about a dozen sites.

ECSS-Projects consist of ESRT (Extended Support for Research Teams) and NIP (Novel and Innovative Projects).

ECSS-Projects has also begun to contribute to the A&D effort. Mark Fahey and Sergiu Sanielevici are developing the use cases and attribute scenarios for High Performance Computing, and Nick Nystrom (PSC, ECSS NIP) develops the use cases and attribute scenarios for Data Analytics with Shawn Strande (SDSC). They have drafted use cases for discussion and review by the architecture team.

Detailed metrics are contained in the individual reports below.

ECSS's Project Managers (Karla Gendler and Natalie Henriques) have continued their tasks of maintaining spreadsheets for project requests, active projects, project assignments and staffing. They continue to review and track workplans, entering staff allocations on each project and quarterly objectives into the spreadsheets. They manage and attend ECSS meetings and XSEDE project management (PM) meetings, posting notes and action items to the ECSS wiki once the meeting has concluded. They provide ECSS information to the XSEDE PM office and relay information from the PM team to ECSS. They also maintain the ECSS wiki and mailing lists. They coordinated the gathering of information for the Q6 report and have published all of the information to the wiki. Using some of TACC's unspent funds, a temporary hire was put in place to aid in transferring all the data from the numerous spreadsheets to Sciforma. This data transfer will be complete in Q1 of 2013. Gendler met with Mike Northrup and Justin Whitt while at the Quarterly Meeting in Florida and spent an extra day testing, working on, and demoing Sciforma

5.0. Testing and customization continues on the software as the PM team is working to make it usable by XSEDE staff.

6.2 ESRT 1.4.1

An ESRT project is a collaborative effort between an XSEDE user group and one or more ECSS staff members, whose goal is to enhance the research group's capability to transform knowledge using XD resources and related technologies. Typical ESRT projects have a duration of several months up to one year and include the optimization and scaling of application codes to use 100,000 nodes or more per job; aggregating petabyte databases from distributed heterogeneous sources and mining them interactively; or helping to discover and adapt the best work and dataflow solution for simulation projects that generate ~100 TB of persistent data per 24-hour run. The first year of the XSEDE ESRT program is also managing projects transitioned from the TeraGrid ASTA program, and all of the ASTA projects will be completed by the end of June 2012.

A request for ESRT support is made by the principal investigator (PI) of a research team via the XSEDE resource allocation process. If the request is recommended by the reviewers and suitable to be an ESRT project, and if staff resources are available, a statement of work for up to one year will be developed by in collaboration by the PI, the ESRT team leader, and the ESRT manager and project manager. The work plan will include staff assignments from the pool of available advanced support experts who have the necessary skills. The ESRT team leader, working with the ECSS project manager, will be responsible for project tracking and reporting and for requesting additional resources or assistance from XSEDE management as needed.

Metrics that quantify ESRT requests this quarter and total active projects are provided in Table 1 and Table 2.

Table 1 ESRT project metrics for this quarter

Metric	**XRAC**	**Startups/Edu**
Number of requests	7	6
Number of projects initiated	7	6
Number of work plans completed	0	2
Number of new work plans completed for previous quarters	4	1

Table 2 ESRT project breakdown

Metric	**XRAC**	**Startup/Edu**
Number of active projects	30	24

As of January 2013, there are 15.54 FTEs assigned to ESRT from NCSA, NICS, PSC, SDSC, and TACC.

Table 3 summarizes the number of requests, unjustified/rejected requests, workplans completed (and as such projects in progress), and work plans still in process. All projects are contacted within the first week or two of being notified of getting recommended for ECSS support.

Table 3 ESRT project metrics since XSEDE began.

	Requests	**Not justified**	**Workplans completed**	**In process**
Jun-Aug startups (2011)	12	8	4	0
Aug XRAC	10	2	8	0
Sep-Dec startups	12	9	3	0
Dec XRAC	11	6	5	0
Jan-Mar startups (2012)	11	4	7	0
Mar XRAC	13	6	7	0
Apr-June startups	12	9	3	0
June XRAC	11	5	5	1
July-Sep startups	9	1	5	3
Sep XRAC	7	3	4	0
Oct-Dec startups	6	-	2	4
Dec XRAC	8	-	0	8
Totals	**122**	**53**	**53**	**16**

For the first 18 months, there has been one main challenge with managing the ESRT program - the management of projects and people. ESRT has a large distributed staff and many different projects with different start/end dates. The project management staff is excellent and has helped tremendously, but we eagerly await the project management software to replace email and spreadsheets.

The following sections highlight a few projects that provide examples of the kind of work that is being done in the ESRT program.

6.2.1 *Improving CFDLib Performance and Scalability (Ogden, UCSD)*

ECSS Project Team: Amit Chourasia (UCSD)

Eruptive conduits feeding volcanic jets and plumes are connected to the atmosphere through volcanic vents that, depending on their size and 3D shape, can alter the dynamics and structure of these eruptions. The host rock comprising the vent, in turn, can collapse, fracture, and erode in response to the eruptive flow field. This project uses cutting edge visualization to illustrate and analyze results from fully coupled numerical simulations of high speed, multiphase volcanic mixtures erupting through erodible, visco-plastic host rocks. This work explores the influence of different host rock rheologies and eruptive conditions on the development of simulated volcanic jets.

Chourasia and Ogden worked to extract and analyze more detailed, quantitative results from the simulations. The main goal of this work is to understand the tightly coupled interaction between jet dynamics and crater growth. This suite of visualization efforts focused on quantifying each of these processes. Specific work conducted during past quarter was:

a) Visualizing cross section slices at various depths for six different variables for temporally varying 9 simulation datasets,

b) Computation of plume area at a given cross section depth for all 9 simulation datasets,

c) Plots of crater growth profiles for all 9 simulation datasets,

d) Topography of plume boundary at last timeset for all 9 simulations

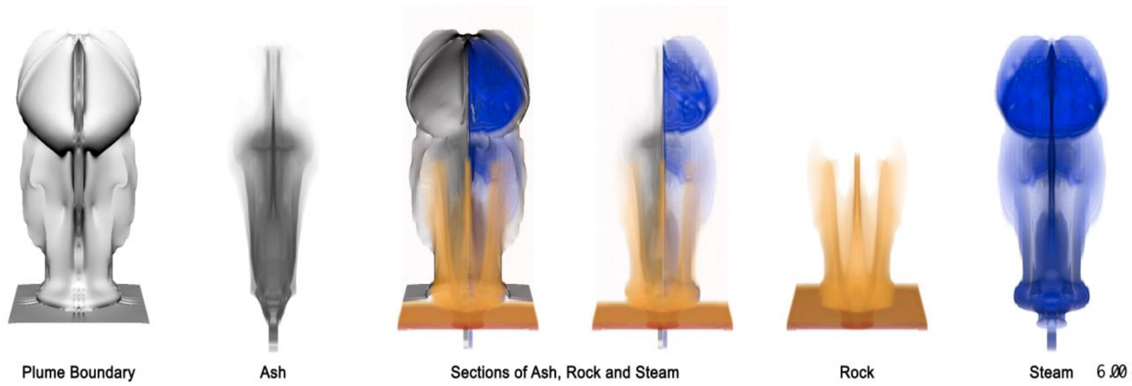


Figure 1 The image shows major components of volcanic eruption based on a simulation with initial conditions of Hi Viscosity and Eruption Pressure at 25 time atmospheric pressure at six seconds. The left inset shows Plume Boundary - a virtual boundary that encompasses all eruptive material inside it ; second inset from left shows volumetric rendering of Ash; right most inset shows volume rendering of Steam; second inset from right shows volume rendering of Rock fragments. The center two insets show the combination of steam and ash in the rear two quadrants and rock in the front two quadrants with and without plume boundary in the back. These visualizations enable us to understand the volumetric distribution of ash, rock and steam in isolation as well as in each other's context for a volcanic eruption. **Credit:** Amit Chourasia (SDSC) and Darcy Ogden (SIO), UCSD.

The PI has indicated that "These snapshot visualizations have been very useful for identifying key dynamics important to studying eruption physics."

6.2.2 Algorithms for behavioral and gas discrimination using artificial sensor arrays (Huerta, UCSD)

ECSS Project Team: Bob Sinkovits (SDSC)

The PI's laboratory has developed algorithms for time series classification of gases and concentration estimation. This project aims to develop fast, scalable and highly optimal versions of these time series classification algorithms. Two goals of this project that have been addressed are (1) to develop optimized, parallel version of software and (2) to improve parallel scalability.

In particular, modifications were made to Ramon Huerta's autoregressive kernel application to achieve better performance. As originally written, this was a serial application. The executable was built using the GNU C++ compiler (g++) and linked the default version of the LAPACK library. Through a combination of compiler, compiler option and library changes together with minor modifications to accommodate modern LAPACK calling conventions, we were able to achieve a speedup of 46x relative to the original code on a single Gordon compute core. A further

3.6x speedup was realized through substantive source code changes, resulting in a total speedup of 167x. We had originally anticipated developing a distributed memory version of the code using parallel linear algebra libraries, but this may not be necessary given the dramatic reductions in run times using a shared memory approach.

Table 4 Summary of performance improvements for ARsym code. All timings obtained on Gordon, and speedups relative to original serial code run on a single Gordon core.

Notes	cores	Run time	Speedup
Original code, GNU compiler	1	11:22:00	-
Switch to Intel compiler and enable AVX	1	05:41:49	2.0
Link threaded MKL library, run in parallel	16	00:14:46	46.2
OpenMP directives in loops in kAR and kARtest	16	00:13:10	52.5
Remove duplicate call to kARtest	16	00:07:58	85.6
Optimization of DYSRK operations	16	00:04:04	167.7

6.2.3 Large eddy simulations of extended wind farms, and direct numerical simulation of turbulent channel flow for a public database (Meneveau, Johns Hopkins)

ECSS Project Team: David Bock (NCSA)

This project studies the interaction between large wind farms with multiple wind-turbines and the atmospheric boundary layer flow. Because the wind-turbines are placed relatively close together their operation and power production is influenced by the wake created by upstream wind-turbines. The simulations, in agreement with field experiment data, show that power production of wind turbines placed downstream of other turbines can decrease up to 50% with respect to the power produced by free standing wind-turbines. Since this decrease is quite substantial, one of the science goals is to use the simulations in order to understand these effects better. The simulations can also be used to test flow structures and how they depend on the design parameters of the wind farm. XSEDE-ECSS goals are to provide assistance implementing two dimensional domain decomposition and parallel FFT as well as 3D visualization representations to assist in simulations and analysis of large wind farms.

To date, this project has designed, developed, and documented multiple visualization scenarios as possible candidates for high-quality production visualization and is now awaiting feedback and comments from researchers. Results can be found in the project webpage link, with representative images below.

http://lantern.ncsa.uiuc.edu/~dbock/Vis/WindFarm/

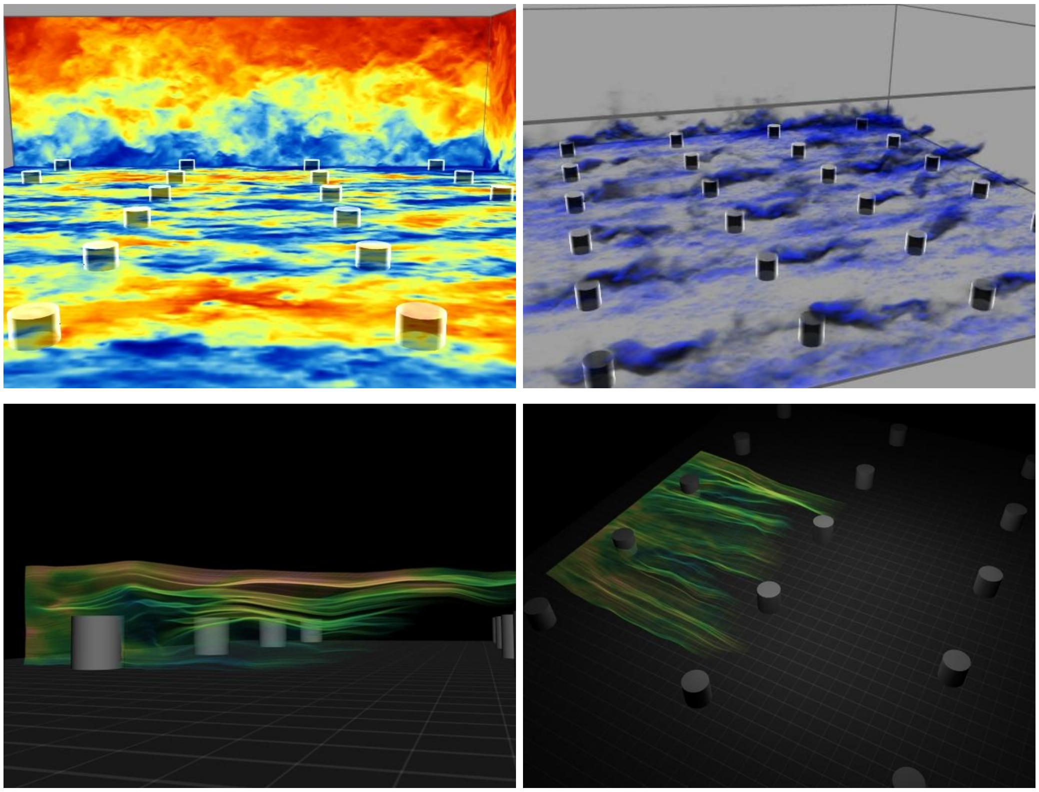


Figure 2 Interaction between wind farms and the atmospheric boundary layer flow

6.2.4 *Effects of Extreme External Conditions on Turbulent Structures in a Boundary Layer (Araya, Texas Tech U.)*

ECSS Project Team: Vince Betro (NICS)

This project has two primary deliverables: (1) to optimize code and I/O to assure that 10,000+ core runs of real-world cases are possible and (2) to perform production runs at very high Reynolds numbers (approximately 15,000 or higher based on the momentum thickness and freestream velocity). To accomplish this, several intermediate goals were identified including profiling, scaling improvements by fixing both IO and communication, and assure production runs at high Reynolds numbers can be performed.

Since this project is relatively new, only some of the milestones have been addressed to date. In particular, profiling has been underway using CrayPAT. Several pieces of information have been identified:

1) I/O is not taking up even 1% of the total execution time, and as such it is not a major stumbling block nor do any significant changes need to be made to the routines.
2) MPI is taking 57.7% of execution time with 47.3% spent in ALL_REDUCE, 7.5% spent in WAIT_ALL, and 1.5% spent in BCAST. The team will be looking for ways to aggregate and re-route some of this communication so that processors can do useful work instead of being in a wait state so much of the time.
3) There are nine routines that take up 33.5% of execution time (seen in Table 1), which were traced during a second profile. All of these routines are highly computationally

intensive linear algebra routines, and as such threading may be looked into in order to speed up some embarrassingly parallel components. A visual description of this initial report can be seen in Figure 1, which was generated by Apprentice2.

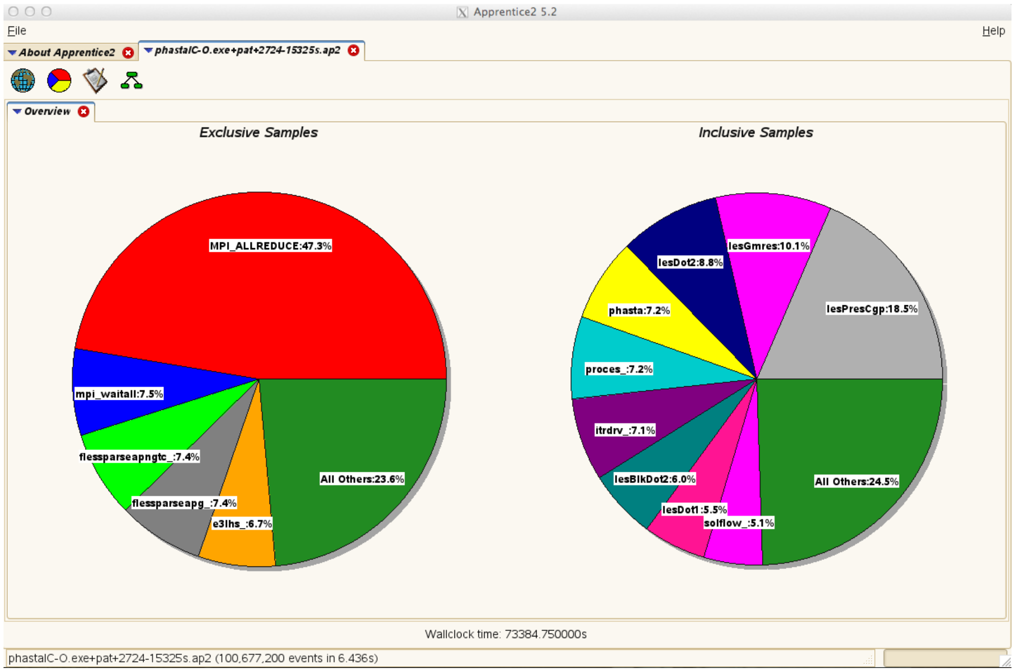


Figure 3 Apprentice2 visualization of time spent in various routines of Phasta

Table 5 Nine routines in Phasta that amount to the top one third of computation time

Percentage of total execution time	User-defined routine
7.4%	flessparseapngtc_
7.4%	flessparseapg_
6.7%	e3lhs_
2.6%	flessparseapkg_
2.2%	fillsparsei_
2.0%	fmtxblkdmaxpy_
2.0%	fmtxblkdot2_
1.9%	fmtxvdimvecmult_
1.3%	flessparseapsclr_

4) Additionally, CrayPAT made the following suggestions on the reinstrumented run. The first suggestion about rank placement seems as if it will bear the most fruit, as it would cut down by 10% the amount of time spent in MPI communication that is almost 50% of the full execution time.

6.3 Novel and Innovative Projects 1.4.2

The mission of the Novel and Innovative Projects (NIP) team is to provide proactive efforts to develop and sustain XSEDE projects by non-traditional (to HPC/CI) users. Activities range from initial contact to the conception and execution of successful projects, including those that receive extended collaborative support. The scope of NIP includes disciplines whose practitioners have rarely availed themselves of HPC/CI resources in the past. It also includes demographic diversity, such as researchers and educators based at MSIs and EPSCoR institutions, and SBIR recipients. Bringing these communities to XSEDE leads to the consideration of applications and programming modes that have not been the focus of HPC in the past, such as those necessary for data analytics and informatics, and of innovative technologies such as streaming from instruments, mobile clients, and the integration and mining of distributed, heterogeneous databases. The implementation of campus bridging processes and technologies will be particularly important for these communities.

Biweekly teleconferences and the use of the project wiki and email list have been successful in catalyzing communications among team members, who benefit from each other's contacts and expertise and share best practices.

It is essential to the XSEDE mission of developing a comprehensive national cyberinfrastructure that we efficiently communicate our experiences in exploring the needs of non-traditional communities to the entire project team. To enable this, we have built a close connection between NIP and the XSEDE systems engineering, user engagement, and technology investigation services. Systems engineering staff now attend each of our biweekly NIP teleconferences and take note of the feedback our team members pick up from the potential and current users they contact and mentor.

In late November, we decided to structure the team into eight "task forces", with 2 or 3 members each. They are: *Minorities; Genomics; Humanities, Arts and Social Sciences (HASS); Economics; Databases & Data Analytics; Geographic Information Systems (GIS) & Visualization; Matlab/Python/R/Java*; *Campus Bridging & Cloud Bridging.* Thus, some team members will focus on understanding and meeting the requirements of specific communities and disciplines, while others will focus on developing and sharing expertise in specific technologies that are likely to be required across communities.

Since the beginning of the program (July 2011), the NIP team (5.5 FTEs) has initiated and executed 30 outreach events; engaged 54 groups of potential XSEDE users; and mentored 72 XSEDE user groups. Team members are currently involved in the technical execution of 10 ECS projects and were involved in 4 ECS projects that were completed by December 31, 2012. They are leading the planning of 5 possible future ECS projects recommended by reviewers.

An important activity has been our workshop "Extending High Performance Computing Beyond its Traditional User Communities" at the 8^{th} IEEE International Conference on eScience in Chicago, see http://www.psc.edu/index.php/escience-2012-workshop for the agenda and the presentation slides. Not counting XSEDE staff members, we had 29 participants from 6 countries. Seven of the presentations report on work done on XSEDE resources with assistance from NIP staff.

We discussed examples of successful projects as well as barriers and suggestions for overcoming them. The main points are:

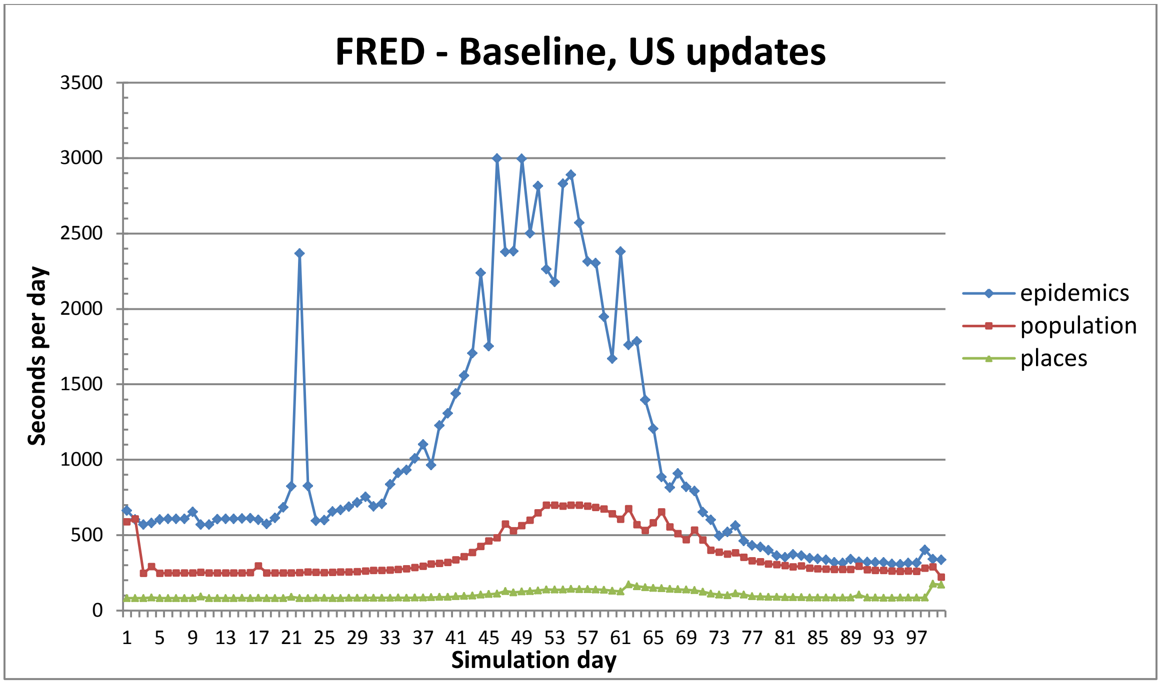
- Need for intuitive interfaces formulated in a given community's language, along the lines of a Gateway, mapping efficiently to the advanced computing infrastructure "behind the scenes".
- Need to use various types of advanced computing infrastructure as seamlessly as possible: local/campus, commercial cloud, XSEDE.
- Many applications are data-centric, and require numerous interactive tasks using persistent storage. Can XSEDE SPs run their big data analysis resources in an interactive, on-demand manner?
- XSEDE needs to figure out how to host data collections, enabling community access and analysis.

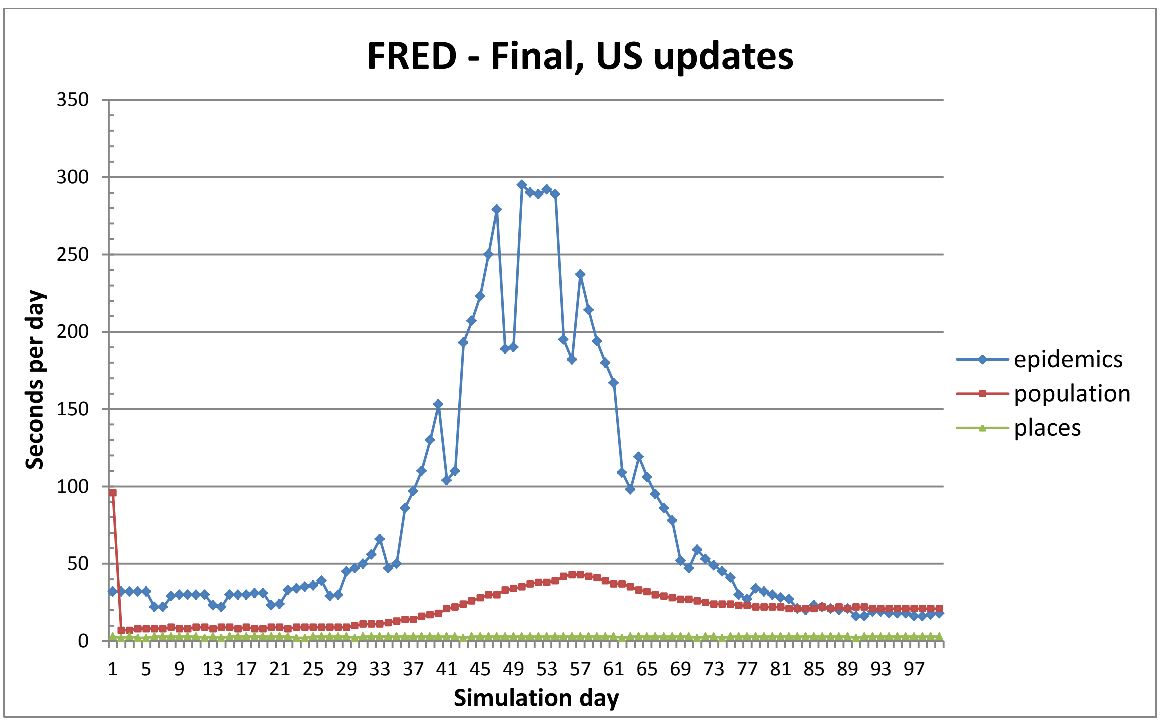
We took these findings into account when defining our NIP task forces, described above.

One of the first four ECSS Campus Champion Fellows, Dirk Colbry of Michigan State University, is a member of the team working on the NIP-supported ECS project *"Interactive Large Scale Media Analytics"* (PI Virginia Kuhn, USC). Dirk is helping to install the multimedia content management software system *Medici* (*medici.ncsa.illinois.edu)* on Gordon; he also developed an annotated bibliography of video analytics software. He is now testing color video analytic software to see what would be helpful, and then integrate the resulting software into *Medici*.

An example of a successful project helped by NIP is *"Computational Explorations in Population Level Disease Spread using Agent Based Modeling"*, with both the XRAC grant's Principal Investigator (Shawn Brown, University of Pittsburgh and PSC) and the ECS consultant (David O'Neal, PSC) members of the NIP team. The context of the project is described in the talk given by John Greffenstette of the University of Pittsburgh at the abovementioned eScience workshop in Chicago, see "FRED Navigator: An Interactive System for Visualizing Results from Large-scale Epidemic Simulations". At the beginning of this project, in December 2011, the computational engine of the FRED software system was fairly limited because of the fact that it was a serial code, in need of both parallel and serial optimizations and requiring large amounts of memory to run even small simulations. The consultant, O'Neal, collaborated with the project programmer, Jay DePasse, at the University of Pittsburgh to improve the serial performance of the software, reduce its memory footprint, and provide OpenMP parallelization. These improvements have significantly enhanced the work that can be done with FRED, by reducing the time to solution, and by enabling larger, more relevant simulations, such as influenza spread throughout the entire US. The research team is now able to evaluate multiple scenarios very quickly, allowing them to provide more accurate and timely decisions for controlling pandemic disease spread. The potential for wide distribution of the FRED simulation software also improved, since hardware requirements for the largest test cases were reduced to near-desktop levels.

The figures below show simulation timings on the PSC Blacklight system, for the entire US, at the beginning of the ECS project ("baseline", January 2012) and at its conclusion (October 2012). The original serial implementation required approximately 96 hours and 540 GB of memory to complete a 100-day US simulation. The current version completes the same analysis in 3 to 4 hours using less than 200 GB of memory. The University of Pittsburgh team has now successfully taken over the further development of the code: another halving of daily run times due to improvements in multithreading is anticipated within a few months.


FRED - Baseline, US updates
Seconds per day
Simulation day
epidemics
population
places


FRED - Final, US updates
Seconds per day
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epidemics
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places

7 Extended Collaborative Support Service – Communities 1.5

7.1 Overview

ECSS Communities focuses on collaborations that impact large numbers of users – those using community codes, those using science gateways and those benefiting from XSEDE's education, outreach and training activities. Gateway use continues to grow significantly. Over 6 million CPU hours on XSEDE resources were consumed by 1629 unique end gateway users or over 42% of all gateway users. This continues the growth over of time of gateway users as a percentage of total users (Figure 7-1).

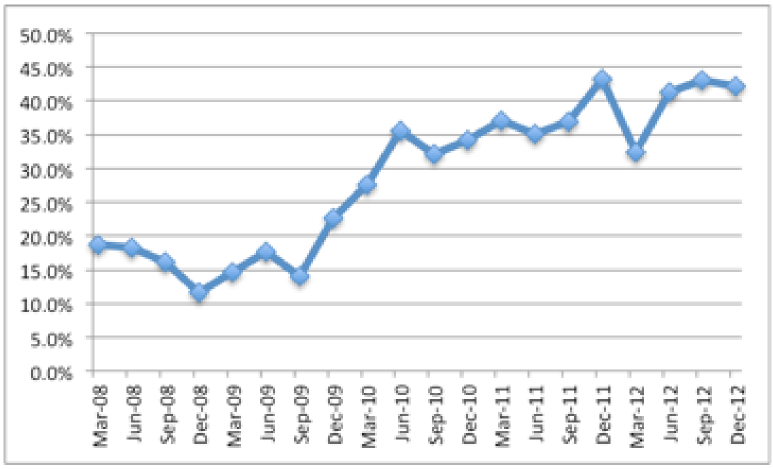


Figure 7-4 Percentage of TeraGrid/XSEDE users who access the resources via science gateways.

This quarter was also active for outreach, featuring presentations at SC12 and tutorials anticipating the arrival of the Stampede system at TACC.

16 ESCC projects and 15 ESSGW projects are currently in progress. In addition to the user-requested projects, ESCC and ESSGW staff continue with internally initiated projects such as optimization and development of commonly used community codes and work on gateway use cases for the XSEDE architecture team.

ECSS staff are significantly involved in the XSEDE13 conference filling key roles in the organizing committee including general chair, chair of the technical program and chairs of several of the technical tracks and visualization showcase.

The ECSS Symposium continues each month and is open to the public to highlight work going on in ECSS projects and allow ECSS staff to learn from one another. The topics this reporting period were:

- Humanities Computing on XSEDE. Presenter: Alan Craig (NCSA)
- Accelerating Cybershake Calculations on Heterogeneous Archetectures. Presenter: Yifeng Cui (SDSC), PI: Thomas Jordan (USC)
- Computational Explorations into Population Level Disease Spread Using Agent Based Modeling. Presenter: David O'Neal (PSC), PI Shaun Brown (University of Pittsburgh)
- Realizing the Universe on XSEDE: Simulation Support for the Dark Energy Survey. Presenter: Raminder Singh (Indiana U), PI August Evrard (U Michigan)

The symposium audience includes the user community, Campus Champions and staff.

In August, 2012 an expression of interest was posted to XSEDE news to gauge interest in the co-allocation of PRACE and XSEDE resources. The thinking was that collaborative work between the US and UK could be pushed forward if teams had coordinated access to a computing resources, allowing them to plan research activities. Several members of the ECSS and PRACE teams developed documents for the PRACE Scientific Steering Committee meeting in mid-January. One document provided a high level view of the benefits of such co-allocation. The second described a more nuts and bolts approach to how requests would be evaluated and processed. As of this writing the PRACE Board is considering these documents at their February meeting.

7.2 Extended Support for Community Codes 1.5.1

Extended Support for Community Codes (ESCC) efforts are aimed at deploying, hardening, and optimizing software systems necessary for extensive research communities to create new knowledge using XD resources and related technologies. ESCC projects are focused on helping users with community codes and tools on XSEDE systems.

Over the past quarter, four new ESCC projects were requested, one was related to a startup request, and the other three were associated with the fourth quarter XRAC allocation requests. In addition to these requests, there were two XRAC renewal projects that requested renewals for previous ESCC projects. Also, there was another request for assistance with the Trinity code on Blacklight. This request will be folded into the Genomics Community Capabilities project. There were no XRAC requests for ESCC.

The startup request proposes to use agent based modeling on Blacklight to simulate the spread of infectious disease. The request is for assistance in scaling up to use a large shared memory system.

Two of the XRAC requests concern climate modeling. Both projects are using the Community Earth System Model (CESM) in different ways. One project is implementing a new ice/land model, while the other is using a modified physics model in the Weather Research and Forecasting Model (WRF) with CESM. Both groups have requested assistance configuring and building their versions of CESM.

The fourth new project involves the implementation of a new boundary condition, (Glide Boundary Conditions) into the AMBER molecular dynamics code. This boundary condition will allow AMBER to better model transport across a membrane. AMBER is one of the most popular community codes within XSEDE.

Over the past year, most requests for assistance for community codes fall under two areas: molecular dynamics and genomics. ESCC will continue to support these areas by initiating new projects to support installed MD codes and genomics workflows. Also, we will investigate the inclusion of CESM as an installed community code on XSEDE systems.

7.3 Extended Science Gateways Support 1.5.2

The Extended Support for Science Gateways (ESSGW) is tasked to provide assistance to researchers wishing to access XSEDE resources through web portals and science gateways. The group assists both new and advanced groups and has experience in the use of web technologies, grid software, fault tolerance, complex workflows, and security and accounting aspects of the program.

Key activities for Science Gateway Program this quarter:

- This quarter a total of over 6 million SU's have been charged through gateway community accounts account from 45,257 jobs. These jobs were executed on behalf of 1629 unique end users.
- Continued organization of interleaving biweekly gateway community and developer meetings.
    - The biweekly gateway symposia on gateways and gateway-related efforts included presentation on cybersecurity from Von Welch, the MyHadoop work at SDSC, and the Computational Infrastructure for Geodynamics Seismology Portal by Eric Heien.
    - The gateways staff calls occur on alternating weeks and focused this quarter on use cases and common middleware requirements, discussed in more detail below.
- The ESSGW effort during this period devoted significant effort to the Science Gateways and Scientific Workflow use case discussions with the XSEDE Architecture and Design team. The use case gathering exercise resulted in an extensive informal questionnaire survey of gateway architecture in regards to XSEDE integration. The effort was coordinated through contributed use cases from teleconferences.
- Initiated a gateway community documentation exercise in developing a gateway cookbook with recipes of various gateway building exercise. This quarter focused on laying out an outline agreeable to all gateway contributors. For reference, the outline and timeline is described at - https://docs.google.com/document/d/1sv2XjHW-Q41KqKgEF-tSLSo1ZcdCLIwimSK3ELm_tbg/edit#heading=h.u87mnyd8s3dp
- Submitted two new areas of gateway focus to XSEDE Management for unspent funds consideration. The group proposes to:
    - Develop gateways for popularly used community codes in order to meet the NSF mandate of broadening XSEDE impact through gateways.
    - Bootstrap a Cyberclient community for gateway developers to share codes and experiences in using XSEDE middleware.
- Continued discussions with XSEDE Architects in strategizing gateway transition to emerging XSEDE Architectural components.
- Worked with Trestles Grid Administrators in testing and validating GRAM5 job management service.

Open Science Grid:

During this quarter, the ESSGW staff has focused on interoperability between XSEDE and the Open Science Grid. Yan Liu with assistance from Mats Rynge have published a major update of the XSEDE OSG web document at https://www.xsede.org/osg-user-guide. The staff has released a sample application package to provide ready-to-use education and outreach materials for science gateways to learn the differences between XSEDE resources and OSG with code and script samples and reference implementations. The code package is distributed from a web location: http://www.ncsa.illinois.edu/People/yanliu/codes/sampleapp.tgz and will be included in XSEDE OSG documentation. The ESSGW staff has provided support to the first OSG user group with PI Qaisar Shafi. The project goal was to study scenarios of physics beyond the Standard Model of particle physics. These include Grand Unified Theories, Supersymmetry and also searching for the elusive Higgs boson. The research strategies typically involve scanning the multidimensional parameter space of various particle physics models using different random number generators. This procedure renders their projects quite extensive and requires submitting a large number of jobs.

7.3.1 Highlights from ECSS SGW projects

7.3.1.1 Dark Energy Survey Simulation Working Group

The ESSGW project focusing on a) migrating the workflow execution to Trestles from Ranger because of Ranger's retirement and b) to run production DES workflows. This effort involved testing the Grid middleware on Trestles and resolving differences between the Ranger and Trestles computational environments. Two significant issues needing resolution were module loading and configuration issues to run MPI jobs. PBS jobs only have /scratch folder write permission on Trestles, but for DES applications required creating a shared folder before running the jobs that is used for sharing intermediate input/output files for a set of jobs in a workflow. To resolve this, SDSC system administrators created a special scratch location for DES project to use. The ESSGW consultants also assisted DES researchers with the execution of two production workflows (identified as "Beluga" and "Chinchilla" within the group) on Ranger, which produced 30 TB of data and consumed 600,000 SU's. Data was moved to SLAC for post processing. Production workflow results are made available from SLAC to DES Science Community and published as a catalog for Blind Cosmology Challenge. This work was described in an ECSS-wide symposium presentation by ESSGW consultant Raminder Singh.

Detailed tasks performed include:

- Migration of code to Trestles to run simulation to extend the production scope.
- Tested the code on Trestles and option to utilize 1024 cores to run large simulations.
- Ran into PBS scripts issue with MPI libraries having different syntax to configure such jobs.
- File system issues were reported on trestles compute nodes while running the large simulations.
- Ran 2 production runs on Ranger: Beluga and Chinchilla, which produced 30 TB of data and consumed 600,000 SU's. Data was moved to SLAC for post processing.
- Updated the Gateway Middleware to the latest available general-purpose gateway middleware Airavata workflow. Further the middleware is now hosted on XSEDE Gateway hosting Virtual machines at IU.
- XSEDE Globus GRAM submissions are initiated through a recommended JGlobus library. The jobs managed through this client have seen occasional failures for long running jobs, precise reason could not be determined. Working with TACC Admins and Globus Developers, the temporary resolution was to disable the job cancellation features in the JGlobus Clients. This addressed the failures and moved forward the DES project. But a long term and permanent fix is needed. The problem and temporary resolution are recorded in the XSEDE ticket number # 220803.

7.3.1.2 *VLAB*

The VLAB project provides petascale computations in mineral physics with the Quantum ESPRESSO codes. Summary: VLAB support activities were minimal during this quarter because of the unavailability of the primary VLAB developer. The ESSGW team was able to reach the developer near the end of the reporting period and did make progress on some technical issues described below.

Detailed activities concluded during this reporting period include:

- Continued work with primary VLAB developer on integrating their portal with current version of Apache Airavata Gateway middleware. This will allow VLAB to outsource migration to different XSEDE resources to the ESSGW team.
- Improved the gateway specifying a local file as an input staging URL. The gateway previously only supported GridFTP urls for input file transfers. The effort involved testing local file protocols in the gateway job submission clients.
- Investigating ways to support VLAB on Stampede.

7.3.1.3 Ultrascan

ESSGW assisted the UltraScan team with the transition of its applications and gateway middleware from Ranger to Trestles. This involved significant operational testing of Trestles' middleware, which was documented in several XSEDE tickets. The ECSS consultants also assisted with the maintenance of the UltraScan team's campus bridging middleware.

Detailed activities concluded during this reporting period include:

- Helped to updating XSEDE Incommon certificates on one of local (campus) cluster.
- Helped with following XSEDE failures:
  - Ticket # 221729 : Connection failure to submit a job on Lonestar . There was some firewall issue that disappeared after some time. The consulting TACC administrator was not able to find anything from grid services log files.
  - Ticket # 221441: Could not find unique HPC input file on Trestles. Node was not able to access the file system.
  - Ticket # 223945 : GridFTP transfer failure from trestles gsiftp://trestles-dm1.sdsc.edu:2811/ endpoint. There was some transient issue. SDSC administrators were not able to replicate the issue next day.
  - Ticket # 222312 : GRAM5 service on Trestles was loading incorrect MPI module, causing jobs to fail. SDSC administrators changed the GRAM service configuration scripts to fix the problem.
- Investigating ways to support UltraScan on Stampede.
- Assisted gateway PI on submitting renewal allocation application to April 2013 XRAC Committee.
- Ultrascan Gateway PI Borries Demeler conducted a workshop in India sponsored by Beckman institute. The workshop presented the XSEDE and XSEDE Science Gateways to internal biophysics community. ESSGW consultants assisted the gateway in ensuing the workshop training sessions are monitored in real-time to ensure smooth user experience.

7.3.1.4 Porting ADaM Data Ming Toolkit to XSEDE

This is a startup request. A group at the University of Alabama in Huntsville developed Algorithm Development and Mining Toolkit (ADaM). The ECSS project will investigate the use of XSEDE resources to execute data mining workflows on big data. The requesting team proposes to use the Apache Airavata software for workflow composition, monitoring, and execution and expects the project will help scientists who do not have access to computing resources to seamlessly create, execute and share data mining workflows. The ECSS team will assist the project team in using XSEDE resources to execute data mining applications through simpler gateway interfaces.

Detailed activities concluded during this reporting period include

- Job scheduling per node will allow users to do scheduling per each node of the their workflow. All the scheduling can be schedule in to node level but can be submitted as a single request to the middleware with a single HTTP request rather submitting multiple requests to each application.
- This quarter's effort also focused on integrating a gateway data management with Apache Airavata gateway middleware. The data registry will help catalog all executions performed on XSEDE resources. Current implementation has focused on Ranger cluster but transition to other XSEDE resources is in progress.

7.3.1.5 Einstein Genome Gateway

The ECSS project is now completed. The gateway requested the gateway hosting resources, which was fulfilled. Due to changes to the project team and re-architecture of the gateway middleware, the PI required no further assistance at this point.

7.3.1.6 CyberGIS

During this quarter, the ESSGW team continued to engage two social science domains: culturomics and political science. In culturomics, the heat map analytical service has been used by researchers to study different types of culturomics data, including global twitter data. Results were highlighted at SuperComputing 2012. In political science, a parallel redistricting algorithm has been under development. The scalability of the underlying parallel genetic algorithm library was further improved through large-scale test runs on TACC Ranger. Computational challenge of handling large amount of variables for optimization problem-solving is being investigated. GISolve middleware and the service-oriented architecture were enhanced for CyberGIS Gateway to use the new XSEDE resources allocated to us in this allocation year, i.e., Gordon@SDSC, Stampede@TACC, and Blacklight@PSC.

The following research publications have been produced:

- Wang, S., Cao, G., Zhang, Z., Zhao, Y., and Padmanabhan, A. 2012. A CyberGIS Environment for Analysis of Location-Based Social Media Data. In: Location-Based Computing and Services, 2nd Edition, ed. A. K. Hassan and H. Amin, CRC Press, in press
- Wang, S. 2012. ‚ÄúSpecial Issue on CyberGIS: Blueprint for Integrated and Scalable Geospatial Software Ecosystems.‚Äù International Journal of Geographical Information Science, accepted

- Shook, E., Wang, S., and Tang, W. ‚ÄúA Communication-Aware Framework for Parallel Spatially Explicit Agent-Based Models.‚Äù International Journal of Geographical Information Science, accepted

Next quarter effort will continue to work on the parallel redistricting algorithm for solving large redistricting problem instances. The ESSGW consultants will work with scientists in public health to develop a disease mapping application that exploits both HPC on XSEDE and high-throughput computing resources through XSEDE-OSG resources. We will continue to enhance our middleware services to manage our use of new XSEDE resources, i.e., Stampede@TACC.

7.3.1.7 Galaxy Bioinformatics Platform on XSEDE

This Quarter, the progress of this project has been slow but some incremental efforts have been made.

On October 25th 2012 the ECSS consultants organized a face to face meeting with the Galaxy team (Anton Nekrutenko and Nate Coraor) and demonstrated the following enhancements to the Galaxy tools:

- Globus Online data movement
- Progress on Global Federated Filesystem (GFFS), the installation is now complete and UI work is ongoing.
- CLI remote job submission from the galaxy instance to Blacklight
- Integration with PSC Speedpage monitoring.
- The following ongoing works also have been presented and discussed:
    - Data Supercell
    - Qstat monitoring tool
- Java/Python interface for GFFS data

7.3.1.8 Social Science Gateway

The ECSS consultants continued work to enable execution of two target R scripts on both SSG (campus) and XSEDE (blacklight@PSC) resources. This quarter focused on:

- Improving XSEDE execution from forking on Blacklight login node to a batch queue.
- Developing a Swift wrapper+configuration to be run from within a submitted job: the user submits a SAS job which calls out to Swift to submit jobs to either SSG or XSEDE resources.
- The ECSS consultant conducted hands on training for PI Lars Vilhuber (Cornell).

7.3.1.9 CIPRES

CIPRES code was consuming a great deal of memory (i.e. about 3 times the file size) when users uploaded files. This limited CIPRES to dealing with relatively small input files and caused the application to crash periodically. To fix the problem, the ESSGW consultant rewrote the code related to uploading files (both the web based single file upload and the applet multiple file upload), as well as other parts of the application that were reading input and result files into memory. Some functionality was lost as a result of the change, but CIPRES is more memory efficient and can handle much larger datasets now.

The ECSS Consultant also assisted the neuroscience gateway to enhance capabilities to notify users who haven't used the site recently (probably 1 year) that their jobs and data will be removed. Deletion will occur automatically unless they log in or contact a site administrator.

Improvements have been made to the CIPRES core infrastructure:

- Fixed a Struts bug that was causing stack overflow crashes.
- Fixed the jsp pages that display information about input datasets.
- Added convertEncoding.sh to translate various common text encoding formats to ascii; reject binary uploads on CIPRES. The script is invoked by CIPRES when a user uploads files. Other portals based on CIPRES, can allow binary uploads by modifying the convertEncoding.sh script. R
- Re-implemented database connection pooling for CIPRES with the tomcat jdbc library.
- The gateway is still debugging ongoing gridftp reliability issues. As a temporary solution, switched over to a cross-mounted nfs file system for Gordon and Trestles.
- Designed the CIPRES REST API

7.4 Extended EOT Support 1.5.3

Over this quarter, ESTEO staff have delivered tutorials, papers, posters, talks workshops and birds-of-a-feather sessions, investing a particularly large amount of effort in the influential SC12 conference. They continue as mentors for Campus Champion Fellows and others. Staff have started preparing for XSEDE13 where Amit Majumdar (SDSC) serves as the Technical Program Chair.

One notable tutorial was the very successful Introduction to OpenACC tutorial that was presented from PSC, in October 2012, with satellite labs at a number of sites across XSEDE. XSEDE ESTEO staff provided the on-site support at the various remote sites. The demand was so great that the event will be repeated in mid-January, 2013. John Urbanic (PSC) prepared and presented a significant amount of the course material, with the remainder provided by a presenter from NVIDIA.

Several ESTEO staff, including Marcela Madrid (PSC) and Mahidhar Tatineni (SDSC) assisted in preparations for the on-line version of the Berkeley course on parallel programming, that will be offered in the spring of 2012. This included porting homework problems onto the Blacklight system at PSC, and deploying unified parallel C onto the Gordon resource at SDSC.

During the period, staff provided outreach and training activities at a wide variety of conferences, including the American Institute of Chemical Engineers annual meeting, the Analytics 2012 Conference, and the eScience conference. Several staff, including Haihang You (NICS) and Frank Willmore (TACC) mentored students this quarter. This also included mentoring activities at tutorials, as needed.

ESTEO staff also continue to review web tutorials and provide new content.

The full list of training courses for the period is available online at https://www.xsede.org/web/xup/course-calendar.

8 Education and Outreach WBS 1.6

8.1 Overview

The Education and Outreach (E&O) team is on schedule and making very good progress achieving its goals and objectives engaging and serving the community.

Based on advice from the TEOS Advisory Committee, the TEOS team conducted the first in a series of annual retreats. The retreat focused on improving integration of activities among the TEOS team and with the rest of XSEDE. The discussions are helping to understand and improve workflows among the various teams, and to improve communications internally and externally.

Many members of the E&O team actively contributed to the annual SC12 Conference as committee members, presenters, exhibitors and attendees.

Numerous XSEDE staff, Campus Champions and members of the community are members of the XSEDE13 Conference planning committee. The committee is developing very exciting plans for the Conference to be held July 22-25.

8.2 Education WBS 1.6.1

8.2.1 Introduction

During this past quarter, the education program made progress on several initiatives. We continued our work with several institutions on formal computational science programs and made visits to two new institutions. We presented XSEDE education materials at two national forums – a meeting of the Coalition for Academic Scientific Computation (CASC) and SC12. We also advanced our efforts to create an online version of the Berkeley parallel computing course and to introduce modeling and simulation into the teacher education program at The Ohio State University. We continued to assist with the publication of the Journal of Computational Science Education by maintaining the journal site and providing staff to assemble an issue. We completed work on a new index of computational science education materials based on the competencies for undergraduate and graduate education and began the process of indexing available materials.

TEOS is working with external partners including Blue Waters, the Virtual School of Computational Science and Engineering (VSCSE), PRACE and RIKEN to leverage our complementary efforts.

8.2.2 Assisting with the Creation of Formal Programs

We continued our work with institutions pursuing formal computational science programs. Consultations were made with several institutions to help formulate their curriculum proposals. Those included Clark Atlanta University, Kane University, Montgomery College, Southern University, and Stockton College. Each institution is in the process of creating formal program documents.

In addition to these institutions, new contacts were made with four other institutions. The University of Arkansas revived its interest in a graduate program in computational science. We held a conference call to discuss a potential visit to campus this winter to meet with the faculty there. Central State University in Ohio is a public, minority serving institution in Ohio where we conducted a half-day workshop in October to provide an overview of XSEDE and integrating computational science into the curriculum. A follow-up meeting with the faculty was held in December to solicit faculty that are interested in inserting modeling materials into their current courses. In October, a visit was made to Sinte Gleska University in South Dakota. This is the only four-year native American university. The one-day workshop introduced faculty to XSEDE and computational science. We also met with the K-12 school superintendent to discuss a possible joint two-day workshop for university and high school faculty on using computational modeling in the curriculum. We expect to hold such a workshop in the spring of 2013. Bob Panoff made presentations and held a workshop at University of Mary Washington in conjunction with their initial investigations to create a computational science program there. A colloquium in November was followed by a two-day workshop in December on computational thinking.

8.2.3 Journal of Computational Science Education

The Journal of Computational Science Education (JOCSE) assembled and published Volume 3 Issue 2 during the past quarter. XSEDE funds contributed to this effort by providing staff to maintain the journal website and to assemble the final issue. Other activities to review articles, provide editorial decisions, and solicit articles were contributed by the editors, editorial board, and reviewers.

8.2.4 Presentations at National Meetings

In October, we organized a half-day workshop on computational science education at the invitation of CASC. The workshop included presentations by Jay Boisseau and Steven Gordon with examples of computational science education programs as well as representatives from several other institutions. The presentation solicited interest in the XSEDE education program from several institutions including the University of Arkansas and Rutgers University.

We also participated in the SC12 education program, presenting a three-hour workshop on teaching the course Introduction to Modeling and Simulation. At this session, Steve Gordon presented the entire course outline as well as examples of modeling exercises and projects. Attendees were also introduced to XSEDE resources that can be incorporated into formal courses. Jennifer Houchins and Aaron Weeden from Shodor Education Foundation helped to manage the LittleFe build-out event at SC12.

Bob Panoff delivered a keynote address "Towards a Generation of Parallel Thinkers" at the Oklahoma Supercomputing Symposium in October. The symposium was attended by 261 people representing 26 academic institutions in seven states, 22 commercial firms, 8 government agencies, and 4 non-governmental organizations.

8.2.5 New Course Development

Modeling and simulation exercises were used in the pre-service curriculum for science and math teachers at the College of Education, The Ohio State University. Materials on environmental science and chemistry were tested in the Autumn semester methods course. The results are currently being analyzed to ascertain what changes need to be made in the materials. Once revised, the materials will be shared with other colleges of education and be used by some of the teachers in their student teaching experiences.

Working with our colleagues at University of California Berkeley, Susan Mehringer (Cornell) and Jay Alameda (NCSA and ESTEO lead) and other ESTEO staff, we have made significant progress on preparing the parallel computing course for online use. The computer exercises have been reviewed and partially assessed for running on XSEDE resources. An example module has been prepared and a tentative schedule for full production and teaching the course in spring should be available soon.

8.2.6 Creation of Repository of Education Materials

Our final activity for the past quarter has been involved with implementing a repository for shared computational science training and education materials. A comprehensive ontology of materials has been installed at the HPC University site with the help of the Shodor Education Foundation and is being readied to accept reviews of existing training and education materials.

The repository will allow faculty and students to search for materials based on subject areas as well as the competencies that have been created as part of our educational program activities.

We are working with Blue Waters and the Virtual School of Computational Science and Engineering (VSCSE) to include the array of VSCSE materials that have been created over the last five years. Further, the XSEDE HPC competencies are being used to help guide the development of VSCSE courses for 2013.

8.2.7 International HPC Summer School

We have begun planning for the fourth HPC Summer School in collaboration with Partnership for Advanced Computing in Europe (PRACE) to be held June 23-28, 2013. The RIKEN Advanced Institute for Computational Science (AICS) will be joining the collaboration in 2013 to include Japanese participants in the Summer School. With the additional of Japan, the program is being renamed from the "*EU-US HPC Summer School*" to be the "*International HPC Summer School*".

8.3 Outreach WBS 1.6.2

8.3.1 Underrepresented Outreach

Identification and Promotion efforts have been focused on participation and support of fall conferences, notably the Southern Regional Education Board's Institute on Teaching and Mentoring (SREB), the American Indian Science and Engineering Society (AISES) annual meeting, and SC12.

- Participants at SREB included over 900 minority doctoral and post-doctoral candidates, who expressed a high interest in using XSEDE resources and services in their work. Underrepresented Outreach is following up.
- Dr Subodh Singh and his student Orlana Schmidt, from Sinte Gleska University in South Dakota were sponsored to attend the AISES meeting in Anchorage, Alaska. Orlana presented a research poster at the conference, and Dr Singh presented an introduction to high performance computing, including XSEDE to this audience. Sinte Gleska is the only Tribal University with post-baccalaureate programs. (Poster and presentations are available on request.)
- XSEDE presented a panel session in the Broader Engagement program at SC12 in Salt Lake City, UT in November. Linda Akli (SURA) chaired the session "Big Data and Visualization for Scientific Discoveries", which included a presentation by John Towns.
- Six participants were sponsored to attend SC12: Edmund Ndip (Hampton University), Luis Cueva-Parra (Auburn University), Sederick Rice (UAPB), Baha Mirghani (NCSU), Veronica Vergara Larrea (Purdue), and Rachel Vinvent-Finley (Southern University). Dr Vincent-Finley mentored a team in the Student Cluster Competition, and Dr Ndip has joined to SC13 Broader Engagement committee. Dr Vincent-Finley has also submitted a report of her experience as an SC12 participant. (Report available on request.)

Deep Engagement is pursuing opportunities with universities interested in establishing academic programs in computational science. Discussions are underway with Central State University (Ohio), Clark Atlanta University (Georgia), Philander Smith College (Arkansas), Virginia State University, and Sinte Gleska University.

The Minority Faculty Council has produced their first draft of recommendations for increasing the number and diversity of participants in the computational science community. The E&O team and MFC are iterating for clarification and will forward to XSEDE Leadership once consensus has been reached.

8.3.2 *Speakers Bureau*

In support of Underrepresented Outreach and Campus Champions, the Speakers Bureau participated in information days at:

- National Technical Association (the oldest African American technical professional organization)
- National Organization for the Professional Advancement of Black Chemists and Chemical Engineers
- University of Oklahoma
- Ohio State University
- Michigan State University
- University of Michigan

Upcoming Events

Dates	**Event**	**Location**
January 15-17	Harvard University SEAS Computefest	Boston, MA
February 7-10	Tapia Celebration of Diversity in Computing	Washington, DC
February 14-18	American Association for the Advancement of Science	Boston, MA
February 19-20	Texas Regional Workshop (UTEP)	El Paso, TX
February 28-March 2	Emerging Researchers Network	Washington, DC
Early April (TBD)	Florida Regional Workshop (Florida International University)	Miami, FL
April 11-12	Washington DC/Baltimore Regional Workshop (University of Maryland Baltimore County)	Baltimore, MD
April 25-28	Humanities, Arts, Science and Technology Advanced Collaboratory	Toronto, Ontario, Canada

8.3.3 *Student Engagement*

The XSEDE Scholars Program is continuing their successful webinar series. Recent offerings included:

- Research Methodologies: Involvement in Scholarly Activities, Publishing and Timelines - Dr. M. Brian Blake
- Safe CO2 Storage: Developing efficient models of underground fluid flow - Paul Delgado & Dr. Vinod Kumar
- Mathematica in serial and parallel - Troy Schaudt, Wolfram Research, Inc, Academic Key Account Manager
- MATLAB in serial and parallel - Gerardo Hernandez Correa, MathWorks Engineer
- Statistics of functional brain networks - Manjari Narayan & Dr. Genevera Allen

The webinar series has evolved into two tracks. The traditional track of mentoring and computing skills topics will continue. Additionally, Scholars are being recruited to present student research talks. The idea for this series came from Manuel Zubieta, XSEDE Scholar and graduate student at the U. of New Orleans. He suggested that public speaking is an area that he thinks a lot of graduate students would welcome practice with. Also, one of the most successful activities from both XSEDE12 and SC11 has been the session during which graduate students shared their research with small groups of undergraduate Scholars. Thus, this series highlights the exciting research of XSEDE Scholars how HPC is used to aid their research efforts. In addition, the sessions provide a forum for fellow students to discuss similar research efforts and ask questions about the graduate school experience.

Staff changes at Rice University have impacted the XSP support personnel. Ruth Kravetz has been hired to replace Alice Fisher, who is moving on to other opportunities. Roger Moye, Rice Campus Champion, is also leaving Rice. In the past, the program manager has relied heavily on the advice of Roger Moye, Rice U. Campus Champion. As he is leaving, we will recruit a small cadre of advisors (faculty and staff) to fill in this gap to help plan future computing/technical workshops, short courses, and learning opportunities. Henry Neeman has already agreed to act as one of the advisors to the program, and Scholars will be strongly encouraged to participate in his Supercomputing in Plain English (SiPE) series.

8.3.4 Campus Champions

New Member Campuses
Utah State University
Michigan Technical University
Old Dominion University
Southern Methodist University
Indiana University of Pennsylvania
Northwest Missouri State University

Number of Member Campusess To-Date:
Total of 133 Institutions
44 EPSCoR
10 Minority Serving Institutions (MSIs)
8 both EPSCoR and MSIs
71 Non-EPSCoR and non-MSIs
Total of 178 Champions

Campus Champions were well represented and active at SC12. In addition to a general Champion meeting and a Champions Leadership meeting, XSEDE hosted a discussion on “How to Make XSEDE Easier to Use”. Champions and XSEDE staff had a very productive and spirited discussion about issues that users have raised when getting started or expanding their use of XSEDE resources and services.

Champion Working Groups:

- Outreach to Campus has conducted a brief survey of Champions, to help focus priorities for future activities
- Both the Student and Regional Champion programs are converging on charter documents to define the new programs. Both are expected to roll out before the end of the current plan year.

It was determined that additional support staff is required to adequately address the rapid growth of the Champions program. Using the ECSS consultant hiring process, Dirk Colbry, a current Champion and Campus Champions Fellow from Michigan State University has been hired as a consultant at 50%FTE to serve in this capacity.

Coordinating with Open Science Grid, Kim Dillman (Purdue) is working closely with ECSS and the Open Science Grid (OSG) staff to develop expertise and identify specific areas of collaboration between XSEDE and OSG that should be addressed proactively. A spreadsheet of current OSG allocations has been compiled and the OSG tutorial from XSEDE12 is being revised to serve as a stand-alone online version.

8.3.5 *XSEDE'13 Conference*

The XSEDE13 organizing committees completed the conference website, finalized and distributed the call for participation (in time for distribution at SC12) and posted a draft schedule. The Easychair submission system has been modified to identify student submitters. Planning for the lightning talks and their description in the CFP has been completed. Social event planning has concluded and contracts are in progress. Registration pricing has been finalized ($450/500/550 for early, regular and late registration; $375/425/475 for students). One-day registration will be available once the early deadlines have passed at a cost of $200 for regular one-day registration and $250 for late one-day. The profit and non-profit sponsor prospectuses have been finalized. The hotel and catering contracts have been finalized and the first site visit has been completed. The team has been able to accommodate a request from the Open Grid Forum to co-locate their meeting. SIGAPP in cooperation status has been granted. Hugh Nicholas from the ECSS team at PSC has been brought on board as an advisor in the biosciences. The XSEDE13 team has reviewed and acted on results from the XSEDE12 attendee survey. The majority of speakers have been identified for the panel on biosciences day. The team will next focus on the identification of plenary speakers and publicizing the submission period.

Details are posted at the conference web site: https://www.xsede.org/web/xsede13.

8.3.6 *Extreme Scaling Workshop*

Planning has begun for the seventh annual Extreme Scaling Workshop. This is a joint effort of the Blue Waters and XSEDE projects. The focus for 2013 will be on heterogeneous computing and is tentatively planned for the late summer or early fall of 2013.

8.4 Community Requirements and External Evaluation WBS 1.6.3

8.4.1 *Community Requirements*

TEOS managers made valuable progress with a TEOS retreat in December. This event, recommended by the Advisory Committee, was a valuable opportunity to discuss both the AC and NSF reviews and TEOS managers' responses. The retreat encompassed leads for most of the specific areas of effort within the Level 3 managers' areas, so the larger group participated in re-calibrating efforts to best reflect our objectives, building stronger connections among the TEOS services, creating shared TEOS-wide processes, and prioritizing areas for improvement as we move into planning Year 3.

TEOS Managers held a series of conference calls with the XSEDE TEOS Evaluators to discuss program evaluation and what the contracted external evaluators could provide in terms of formative feedback for future planning. This was a valuable opportunity to clarify the metrics currently being collected, and those that are outside of scope of the external evaluation team.

TEOS Advisory Committee met via conference call on Thursday October 18, 2012. At the 90-minute meeting, TEOS managers presented their responses to the NSF Review, as well as the feedback from the AC meeting on their presentations at the previous meetings. The expanded membership brings in new perspectives, though it complicates finding dates that allow participation by all the committee members.

8.4.1.1 Next Quarter Focus

The next AC meeting will be in person, on February 25-26 in Chicago. At that meeting, we will present outcomes from the retreat, discuss Year 3 plans, and discuss priorities for audience surveys or interviews to support clearer understanding of how to tackle Year 3 initiatives.

8.4.1.2 Risks

TEOS Strategic Planning Retreat recommendations still require prioritization and review by the larger XSEDE leadership team. There are risks of unintended consequences from any proposed changes, but XSEDE leadership team review should identify most of those. Continued communication with XSEDE Level 2 and Level 3 managers should quickly identify and remedy any such unintended consequences. The Community Requirements Manager will work with Scott Lathrop on a communication plan to extend across TEOS and XSEDE to mitigate that risk.

8.4.2 External Evaluation

The external evaluation team was very active working with the TEOS teams described below.

8.4.2.1 Training

The external evaluation team continued to explore the feasibility of tracking users longitudinally through the XSEDE User Portal (XUP). We've hired a graduate student, Michael Culbertson, to work on this task. Michael began working on January 7th, 2013.

During the December TEOS retreat, the evaluation team discussed a number of issues with members of the Training program and TEOS management in order to determine the appropriate next steps. These issues included (1) low survey response rates on the XUP and (2) threats to longitudinally tracking users through the XUP (multiple login IDs and registration outside the XUP). As a result of these discussions the evaluation team discovered multiple surveys from different sources were being used to follow up with participants after training activities. This was primarily due to an instructor lack of awareness of the existing evaluation methods. To address this, the evaluation team will work with training representatives at main XSEDE sites to create standardized surveys for reoccurring training activities and thus minimize the amount of spam towards participants and increase instructor awareness and compliance. Although we expect this standardized survey suite to significantly help with measuring the impact of the training program, the registration and attendance recording inconsistencies from site to site will continue to affect the ability of the evaluation team to do this adequately.

8.4.2.2 Education

Sinte Gleska University hosted an onsite XSEDE Workshop on October 12, 2012. The external evaluation team drafted a short paper and pencil survey that was administered and collected by Steve Gordon on site. The surveys were sent to the external evaluation team for analysis and reporting. 100% (5/5) of workshop participants responded to the survey. 80% (4/5) of the participants classified themselves as "instructors" and most plan on incorporating the classroom models demonstrated by Dr. Gordon into their teaching. Many expressed interest in continuing to learn about XSEDE's services and participate in training/education programs to familiarize themselves with HPC. An interim evaluation report was submitted to Steve Gordon and Scott Lathrop in November 2012 and can also be found on the E&O Evaluation wiki under TEOS Evaluation Reports.

8.4.2.3 Outreach

Student Engagement: A post-participation online survey was administered to student participants of the 2012 XSEDE Student Engagement Program. 60% (9/15) of the students responded to the web survey. 78% (7/9) of students agreed or strongly agreed that the program met their expectations and were satisfied with the interaction they had with their supervisor. 88% (8/9) agreed or strongly agreed with the statement, "I am satisfied with my research experience." 44% (4/9) claim the quality or scope of their research, work, or major has changed since they became involved in the program and 77% (7/9) applied for additional programs, conferences, and/or research opportunities in HPC. An interim evaluation report was submitted to Scott

Lathrop and Laura McGinnis in November 2012 and can also be found on the E&O Evaluation wiki under TEOS Evaluation Reports.

Program supervisors also received a post-participation survey to determine the added-value of participation and offer suggestions to improve the program. 62% (8/13) of supervisors responded to the web survey. Supervisors repeatedly cited gains in their project development, mentoring skills, and collaborations as a result of participation in the program. Recommendations for improvement included increasing the timeframe for student activities. An interim evaluation report was submitted to Laura McGinnis and Scott Lathrop in November 2012 and can also be found on the E&O Evaluation wiki under TEOS Evaluation Reports.

Campus Champions Fellows: The evaluation team conducted interviews with current Campus Champions fellows to document the status of the program and help management increase participation next year. Preliminary findings from these interviews suggest low application rates could be due to a lack of understanding of work/roles amongst the champions in addition to apprehension regarding the additional workload and time commitment. Fellows also expressed a desire for more flexibility in the program. Some would like to take a sabbatical and work full time on the projects while others prefer the current timeframe. All fellows have cited hands-on experience and collaborating with other groups as significant benefits of participation in the program. An interim report will be generated and submitted to program management this quarter.

Minority Outreach: Evaluators are currently engaged in the planning of upcoming regional events. Data from the Nashville Regional Event (May 2012) is being utilized to inform program planning and decision making. Evaluators plan on attending the February 19-20 regional workshop at the University of Texas, El Paso as well as the developing workshops at the University of Maryland Baltimore County and Florida International University. The evaluation team is working with program management to develop a follow up survey and determine what data can be collected for other TEOS programs during these events.

8.4.2.4 Campus Bridging

Evaluators continue to work with the Campus Bridging team to formalize the evaluation plans. Lorna Rivera has attended regular Campus Bridging phone calls to inform evaluation plans. An Indiana University site visit was conducted on October 29, 2012. Lorna conducted individual interviews with Campus Bridging staff during the visit. Following these interviews Lorna conducted a focus group with all of the interview participants to relay and clarify the information that was gathered to the larger group. This was strategically helpful to understanding the goals and next steps for the program. A follow up meeting with Craig Stewart, Scott Lathrop and the Campus Bridging team was held on December 19th, 2012 to further discuss the program's status and evaluation plans. The evaluation team is scheduling an additional meeting to take place early in 2013 to address necessary changes to the evaluation plans as a result of the program's status.

8.4.2.5 Cross Coordination

User Survey and Community Requirements: On October 10th the external evaluation team met with the leads of TEOS's Community Requirements and the User Survey teams, Diane Baxter and Craig Stewart, respectively. During this meeting the external evaluators suggested the standard inclusion of linking questions in XSEDE surveys to allow for data comparisons across surveys. The linking questions center on respondent roles, XSEDE usage, institutional demographics, and individual demographics. The external evaluation team has worked with the User Survey team to include these questions in the 2013 survey as well as provide general feedback on the survey's design.

8.4.2.6 Dissemination

In October the external evaluation team was encouraged to share the TEOS evaluation methods and metrics with the larger community. On October 9th the external evaluation team presented the evaluation plan and metrics to the TEOS community during the all TEOS call. The evaluation team will also present two papers at the Center for Culturally Responsive Evaluation and Assessment (CREA) 2013 conference.

8.4.2.7 Plans for Next Quarter

In addition to the aforementioned plans, evaluators will continue to develop and prepare to implement the longitudinal tracking. The evaluation team will also finalize plans for upcoming TEOS case studies.

8.5 TEOS Infrastructure WBS 1.6.4

Forty-nine distinct events were added to the Education & Outreach Blog on the XSEDE web site. Ange Mason (SDSC) collects and vettes events for their suitability for various components of our intended audiences, and rewrites the introductions as appropriate.

A new Facebook presence was initiated in December 2012 and has begun to be populated with Events and other announcements and items from the E&O XSEDE Blog. The new Facebook presence is independent of the main XSEDE Facebook page, and is entitled Computational Science Education News. The new presence will be pushed out to collaborators and thence through their various outlets into the communities that care about computational science and research in our schools at all levels.

Mason and Jim Ferguson have been working with the Blue Waters project and the HPC University effort to re-design the site and feature a feed from the E&O Blog directly to the HPC University main page. This effort began in the summer with an XSEDE-sponsored student intern at Shodor and has moved on to regular web staff at Shodor. The next bit of functionality to be finalized is a web form for prospective students who are interested in advertised internship opportunities.

Ferguson and Mason continued a process to reorganize the TEOS web presence at XSEDE with calls for comment and new information from the other TEOS area leads. In the interim, text for each subproject is undergoing review and update following accomplishments and changes in plan during this second year of the XSEDE project.

8.6 Campus Bridging WBS 1.6.5

8.6.1 Discussion of Campus Bridging

The Campus Bridging team continued to disseminate information about XSEDE's Campus Bridging via videos produced in the previous quarter: https://pti.iu.edu/campusbridging/what-is-campus-bridging and https://pti.iu.edu/campusbridging/penguin-computing-and-iu. The bulk of Campus Bridging efforts were in the area of moving the GFFS Pilot project forward and in the software packaging projects. One report describing priorities for Campus Bridging in years 2-5 was published, and a detailed plan for cluster software distribution was drafted and disseminated within XSEDE for comment.

8.6.2 GFFS Pilot Project

GFFS Pilot teams met at SC12 in order to answer questions and get individual sites using the GFFS software, as well as to iron out final difficulties using the UVA testbed grid. Campus Bridging teams met with Operations multiple times in order to work through documentation and installation packages. Operations released installers for XSEDE GFFS during the week of 12/31/2012. Texas A&M will be the first pilot site to work with the GFFS software.

8.6.3 *Campus Bridging Software Packages*

The Campus Bridging team has, in concert with Operations and Software Development and Integration teams, put together a list of XSEDE software that is approved for inclusion in the XSEDE Campus Bridging Rocks Rolls and packaged software. Campus Bridging is working to establish milestones for the packaging of the software and a distribution mechanism for users. Campus Bridging continues to work with Operations, A&D, and SD&I to establish a plan for software packaging that pursues XSEDE's strategic goals for making XSEDE services available to campuses using the Campus Bridging software packages. The first phase of software packaging will focus on basic functionality and scientific software, while later phases will pursue tighter integration with XSEDE. Cornell will lead the packaging effort, with volunteers at IU and SURA institutions to test software installation after Operations has tested installation functionality internally.

8.6.4 *Risks*

Campus Bridging anticipates risks in reestablishing enthusiasm in the GFFS pilot sites for working with the software. Some of the sites have been reticent or critical of XSEDE due to the delays in pilot testing, and the Campus Bridging team will need to re-start the pilot process. Little time remains for software packages to be built, tested, documented and disseminated in PY2, and so the Campus Bridging team will need to pursue the software packaging efforts with alacrity in order to complete packaging initiatives before the end of the program year.

9 TAIS/Technology Insertion 1.7

The Technology Investigation Service team continues to make good progress both with the integration into the XSEDE project as well as performing technology evaluations. During this quarter the final phase of the merging of the TIS and XSEDE web sites was completed. The evaluation process in continuing to identify and evaluate technologies that might be useful in XSEDE.

TIS has begun engaging other areas of XSEDE, in particular, the Operations group and the SD&I group. There were two areas of collaboration identified and effort started this quarter. First, a technology evaluation was initiated that will complement work being done in the other two groups. Second, a discussion was held and agreement was reached to better integrate the provisioning of test systems for evaluations across all three groups. Work is ongoing to better define and execute this plan.

In addition to the work with Operations and SD&I, TIS continues to have a close association with the User Engagement team through the participation of Sergiu Sanielevici in the bi-weekly TIS all-hands meetings.

TIS Project Management completed the Program Change Request (PCR) to formally and officially combine TIS and XSEDE.

Finally, work is being done to understand the budget and spending status of the TIS project. The TIS project leadership is evaluating plans for properly and completely using the allocated budget in a way consistent with the overall Statement of Work. This process will continue for the remaining quarters of the TIS project.

Details of the web work and evaluations are below.

9.1 1.7.1 Technology Identification

This quarter was focused on implementing the migration plan to XSEDE infrastructure which was completed. In addition to moving the web and database deployments, the code base for XTED was migrated to Github and integrated with the larger XSEDE code base. With these processes complete, active development can begin in full in Q1 2013.

9.2 1.7.2 Technology Evaluation

The evaluation for Pegasus has been completed and recommended Pegasus for Workflow Management System. The Unicore evaluation is at the testing stage. Chris Koeritz (UVa) left the group and has been replaced by Vana Venkataswamy, also from UVa.

We have started writing the TEP training package, which will be useful for training new members of the TIS evaluation team.

Progress continues on technology evaluations. Test runs were started on the Unicore Evaluation. The re-evaluation of GFFS as a Reliable File Transfer (RFT) service was started and deferred. The capabilities we wanted to evaluate were not available in the current release. XSEDE OPs made a request to evaluate candidates for Two Factor Authentication (OTP). The team is investigating potential technology candidates for its next evaluations.

In the next quarter, we will finish the current Unicore evaluation. We will start and finish the new OTP evaluations. We will finalize the training package for new evaluation team members and train Vana with it.

10 TAIS/Audit Services 1.8: *Technical Progress XDMoD Auditing Framework*

10.1.1 Release of XDMoD 2.5

XDMoD 2.5 was released just previous to SC12. It includes a number of new features and improvements that are described in the subsections below.

10.1.2 Compliance Tab

A compliance tab was added to the XDMoD framework to provide NSF Program Officers and XSEDE leadership with a tool to quickly assess service provider compliance with XSEDE operational reporting requirements. Figure 10.1 shows a snapshot of this feature. The new compliance tab tracks whether or not each service provider is supplying required reporting metrics and data. The metrics are shown in the first column of Figure 10.1. Required metrics (as determined by XSEDE) are shown using a bold face font while additional metrics that TAS strongly recommends should be collected are in the lighter (grey) font. The time frame of the compliance is user selectable, providing a compliance history for the service providers. Like the charts generated with XDMOD, compliance data can be output as a report in the Report Generator using a newly-developed template.

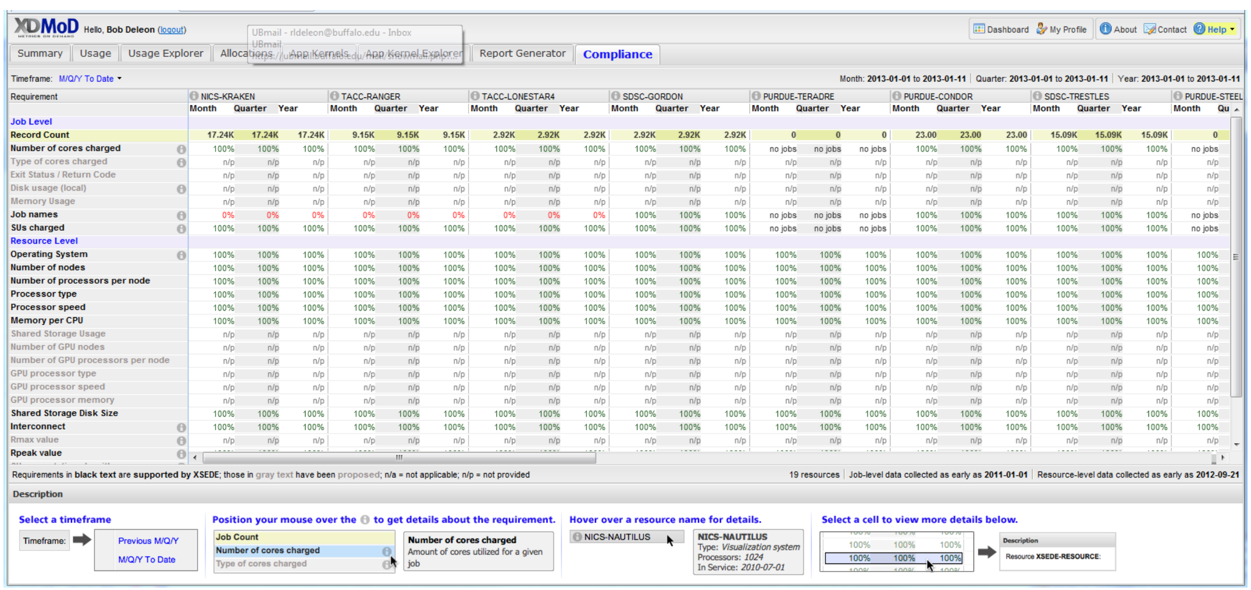


Figure 10.1-1 XDMoD Compliance tab

10.1.3 Application Resource Runner (ARR) software

Software to better manage organizing, submitting, running and tracking the results of the application kernels was developed this quarter. Prior to this, Inca was used for this purpose. However, Inca was not designed to support the deployment of application kernels and therefore it was determined that new software would be needed to improve the reliability of the process and collect information regarding quality of service. The new software, abbreviated ARR, has proven to be more flexible and robust in initial testing. ARR will allow TAS to perform a more thorough statistical analysis of the overall application kernel performance. This study is presently in progress and the results will likely be included in the next quarterly report.

10.1.4 Operations Dashboard Design and Development

XDMoD is a complex application that draws its information from multiple sources and runs several internal processes to support ingestion and aggregation of data from these sources. While some of these data sources are managed directly by the XDMoD team (e.g., the application kernels) many others such as the XDcDB and the POPS database are not. In order to provide a reliable service, it is important that the XDMoD team be able to monitor the health of these data sources, the process of ingesting and aggregating data, and several other internal XDMoD processes. To support this task, we are developing a new operational dashboard that will allow staff to quickly assess the current state of processes within the XDMoD application and take action to rectify any issues. Each internal ingestion process has been instrumented to send log data into the XDMoD data warehouse, in addition to the traditional log file, so that a summary can be provided and potential issues more easily identified from a central location.

This dashboard, initially available only to the XDMoD development team, provides an operational summary of all periodic processes executed by XDMoD. This includes: data ingestion from multiple sources including the XDcDB, POPS, and RDR; the deployment of the application kernels and the ingestion of their data; and the process of mirroring a local copy of the XDcDB from Pittsburgh. Failure of any of these processes may also help to identify issues with the data source itself. For example, a failure in the process of ingesting XDcDB data from our local mirror led to the discovery and subsequent correction of an issue in the mirroring process between SDSC and PSC.

The operations dashboard consists of a summary screen, shown in Figure 10.1-2, which displays an overview of the most recent invocation of each internal process. These currently include a report on active users, data warehouse ingestion, report generation, compliance ingestion, application kernel ingestion, and application kernel deployment. Here we can highlight potential issues that operations personnel should investigate. Clicking on any summary will direct the user to detailed information on each process. For most ingestion processes, this summary consists of the log entries for that process that can be sorted and filtered by log priority (e.g., information, warning, error, etc.), and by date. By default, only the log entries pertaining to the last invocation of the process are displayed but this can be easily expanded by the user. Log entries indicating an error state are highlighted in red and also displayed directly on the summary page.

The application kernel deployment engine (ARR), in addition to providing log entries, maintains the state of all application kernels scheduled to run at the various resource providers including complete logs of run success/failure rates and application output. The dashboard makes use of this information and allows operations personnel to quickly identify failed application kernels and immediately drill down to view error messages and inspect the complete output of the failed kernel. Figure 10.1-3 shows a sample set of application kernel results from Alamo, Gordon, and Edge (a local CCR resource). We immediately identify that WRF is failing on Alamo and

Gordon while Games, Amber, and WRF are running reasonably well on other platforms. We can also drill down to details on individual runs to view complete deployment and application output. In the future we will examine data returned by failed application kernels in an attempt to automatically identify potential causes of failure such as unmounted filesystems or compute nodes common to several failed kernels.

It is anticipated that certain portions of this dashboard will be made available to a broader audience as appropriate so that service providers can utilize data such as the application kernels to assess quality of service and proactively identify potential hardware and configuration issues.

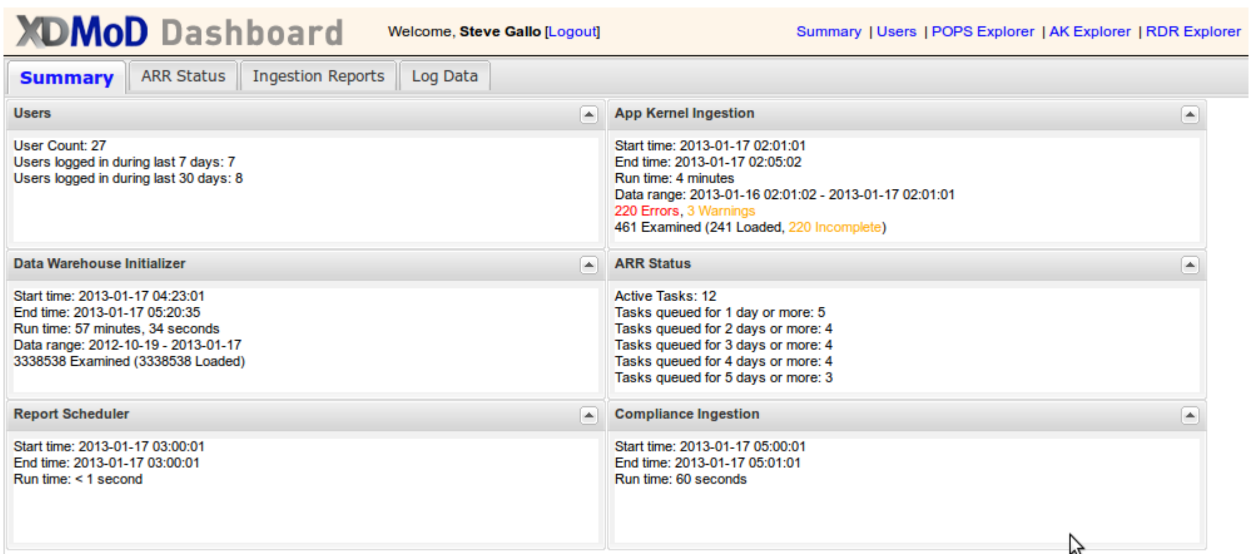


Figure 10.1-2 XDMoD operations dashboard summary

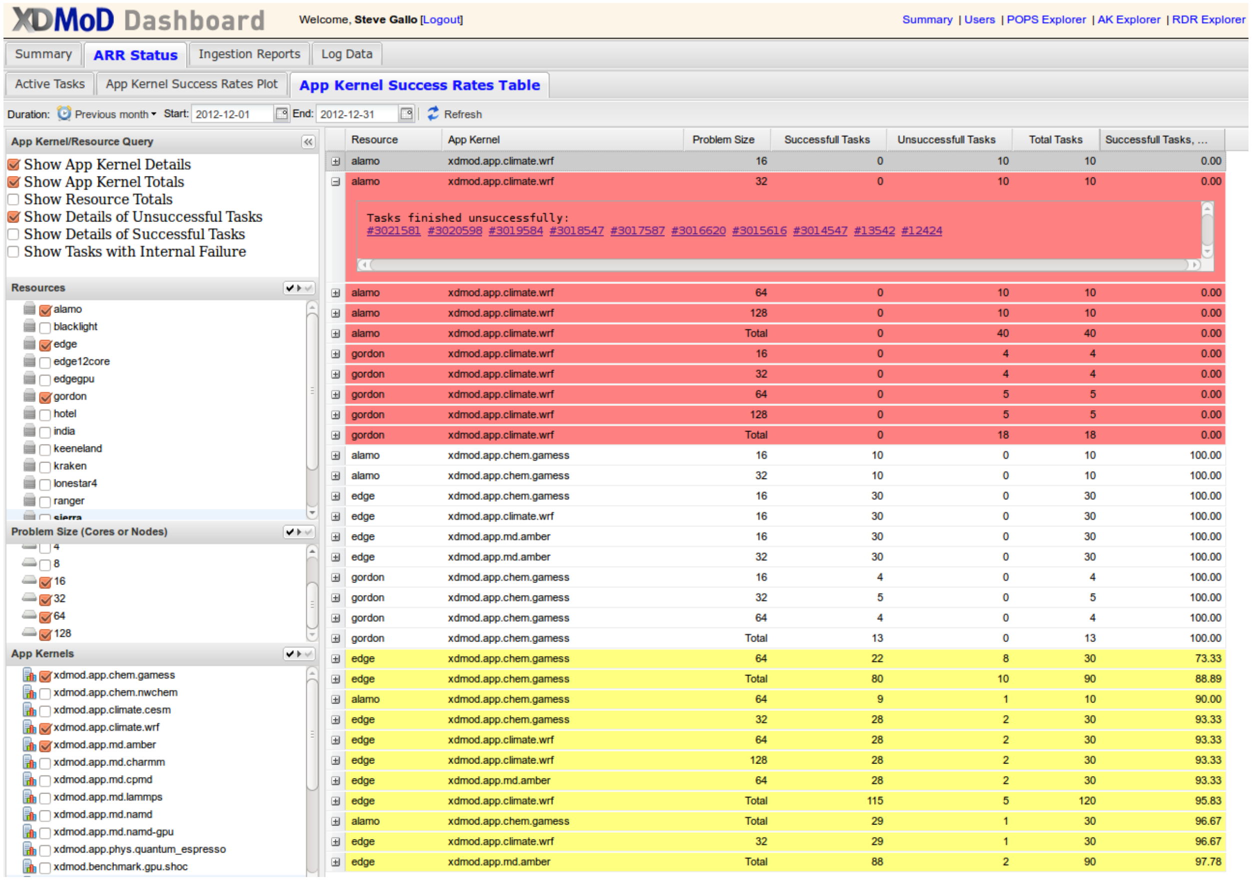


Figure 10.1-3 Application Kernel Deployment Details and QoS

10.1.5 Improvement of POPS Allocation Data Metrics in XDMoD

The Allocation realm in XDMoD has been improved by carefully processing the data from the POPS database and by the addition of more metrics. The XDMoD Allocation realm now tracks: Allocation Burn Rate, Allocation Usage Rate, Number of Active Allocations, Total NUs Allocated, Total core hours (Raw SUs) Allocated, Total XD SUs Allocated and Total XD SUs Used.

10.1.6 Improvements to the XDMoD Custom Report Generator

Based on user feedback, the Custom Report Builder has been improved to both add functionality as well as make it easier to use. For example, as shown in Figure 10.1-4, a user new to the Custom Report Builder is now presented with a detailed description of the various options for adding charts for incorporation into reports. In addition, new service provider quarterly report and compliance report templates have been added to the template pallet. As other useful templates are identified they will also be added.

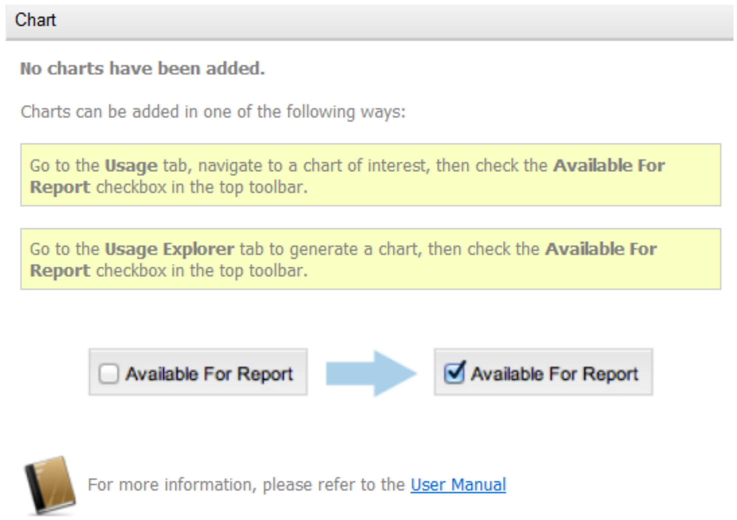


Figure 10.1-4 XDMoD Custom Report Generator view previous to the addition of charts.

10.1.7 Improvements to the XDMoD Summary tab

The XDMoD Summary tab has been greatly improved. First, HighCharts, which is the charting package utilized in the Usage Explorer, is now employed by the Summary tab. Second, the Summary page can be customized to display user selected plots instead of the default plots. This is achieved simply by generating the desired plot using the Usage Explorer and checking a box within the Usage Explorer to have the plot included on the summary page.

10.2 NICS Sub-contract: PEAK progress:

10.2.1. Objectives

In the current reporting period, we extended our work on the PEAK project to include scientific applications, as opposed to kernels with BLAS/LAPACK functions. It is important to optimize configurations for scientific applications due to the following reasons:

1. Most HPC users run applications, not kernels.
2. The configuration of a scientific application is more complex. The installation process of some applications is not straightforward.
3. The run time of a scientific application is usually much longer.

However, the basic idea remains the same; that is, we still build an application with different compilers. In addition, if an application uses numerical libraries, available alternatives on Kraken (i.e., ACML from AMD and MKL from Intel) can be linked, instead of the default LibSci from Cray. FFTW is another possible option for performance tuning. In our study, we have only varied the version of Cray FFTW available on Kraken (i.e., Cray FFTW2 and Cray FFTW3).

These three factors (i.e., compiler, numerical library, and FFTW version) enable us to build a number of versions for each application. Therefore, this number ranges from 1 to 18, theoretically. The actual number of versions of a selected application is subject to: 1) the compatibility of its code with different compilers and versions of FFTW; 2) its usage of a numerical library.

To benefit Kraken users, we targeted the most-used applications on Kraken. In this reporting period five applications were studied: 1) NAMD; 2) LAMMPS; 3) GROMACS; 4) CPMD, and 5) AMBER. Kraken provides only one version for each of these five applications, while our main objective is to produce as many versions as possible and then conduct a performance comparison in order to find the optimized configuration.

10.2.2. Results

Official benchmark tests are downloaded to benchmark each version of an application. The shortest execution time among five trials that a specific version is able to achieve is selected as the performance data for subsequent analysis.

10.2.2.1 NAMD

NAMD does not use BLAS/LAPACK functions. It does need to be linked with an FFTW library but it is only compatible with FFTW2. As a result, the number of versions that we can produce with NAMD is limited. In other words, we can build NAMD only with three compilers on Kraken. Three versions (namd-gnu, namd-intel, and namd-pgi) were built successfully. Unfortunately, namd-pgi did not generate correct output files. Therefore, we gathered the performance data for only two versions of NAMD, as shown in Table 1.

As shown in the two figures below, the GNU version is roughly 10 percent faster than its Intel counterpart in most cases. When 768 cores are utilized, the differences are very small. The performance differences are consistent in all cases.

Table 6. Performance data of NAMD-STMV (unit: second).

	12-core	**24-core**	**48-core**	**96-core**	**192-core**	**384-core**	**768-core**
GNU	8072.58	4059.80	2073.69	1055.56	540.67	284.92	150.99
Intel	8940.70	4488.64	2292.61	1165.06	608.25	312.46	167.20

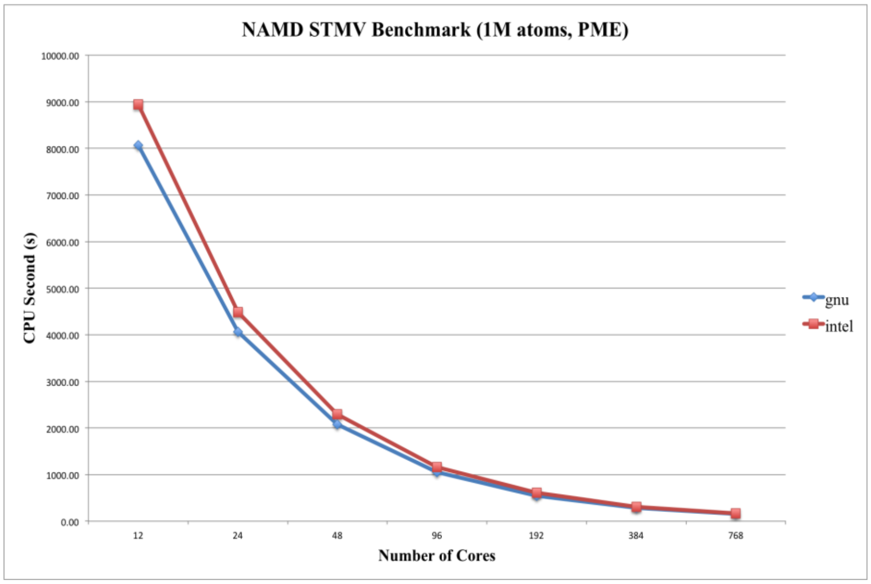


Figure 10.2-5. Performance data of NAMD-STMV.

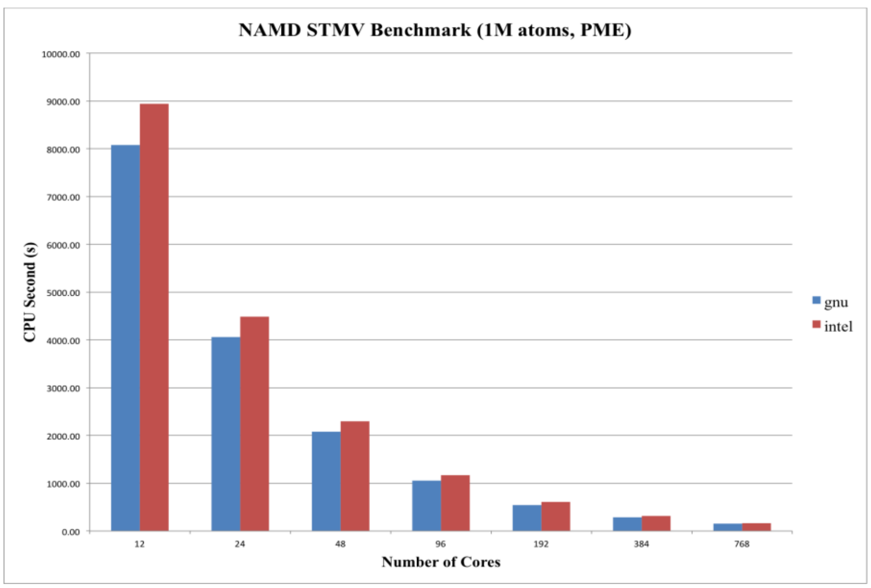


Figure 10.2-6. Performance data of NAMD-STMV.

10.2.2.2 LAMMPS

The configuration with LAMMPS is very similar to that of NAMD in the sense that we do not have any options to tune this application by varying a numerical library or the FFTW library. For this application, we built three compiler versions (lammps-gnu, lammps-intel, and lammps-pgi) as well, as shown in Table 2.

Generally, the GNU and Intel versions have very similar performance, while the Intel version is only slightly faster than its GNU counterpart, as shown in the two figures below. The PGI version, on the other hand, is slower by 20% or so in most cases.

Table 7. Performance data of LAMMPS-RHODO (unit:second).

	12-core	24-core	48-core	96-core	192-core	384-core	768-core
GNU	68.34	34.63	17.94	9.41	4.83	2.72	1.60
Intel	67.74	34.17	17.70	9.07	4.77	2.69	1.58
PGI	83.58	42.50	21.92	11.34	5.80	3.23	1.86

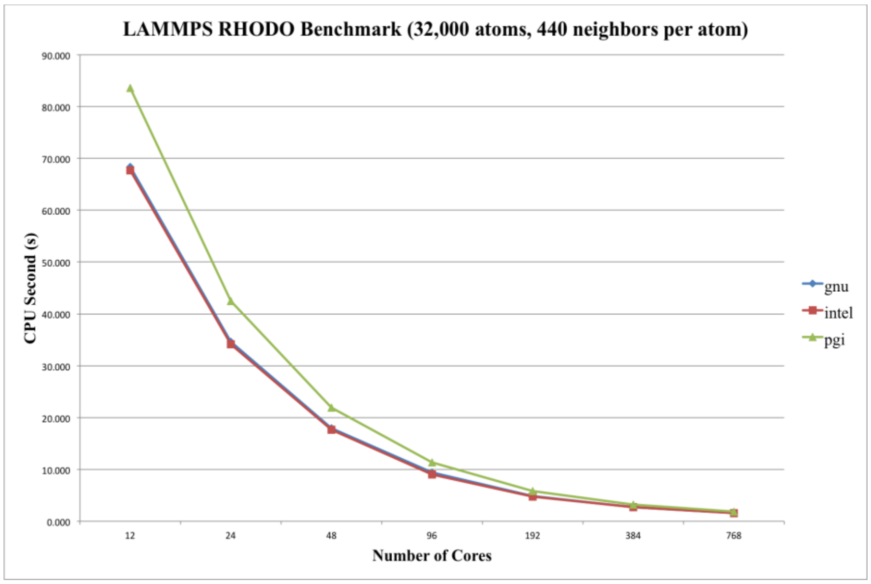


Figure 10.2-7. Performance data of LAMMPS-RHODO.

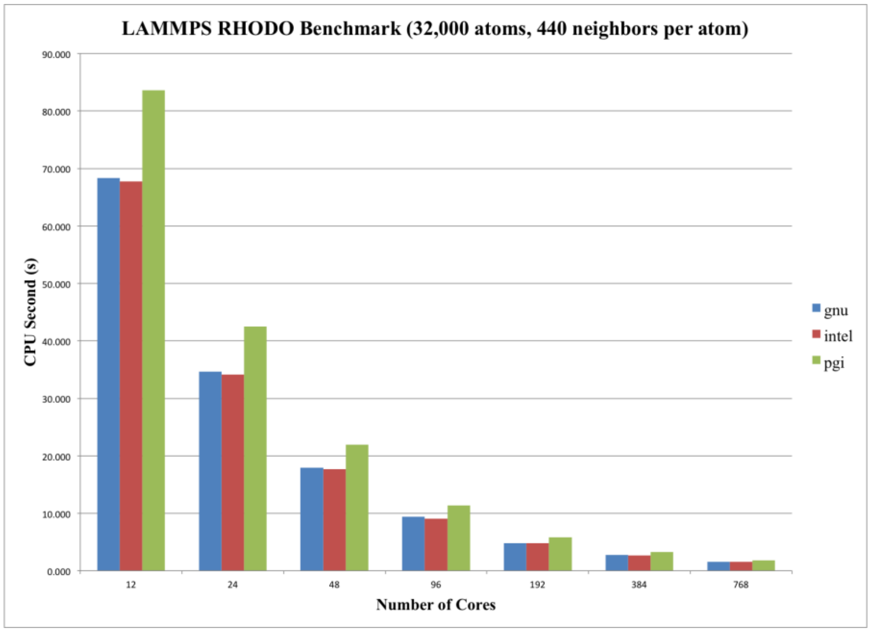


Figure 10.2-8. Performance data of LAMMPS-RHODO.

10.2.2.3 GROMACS

GROMACS uses BLAS/LAPACK functions. On Kraken, LibSci is the default numerical library which will be linked automatically with GROMACS. To find out whether other available numerical libraries would improve or degrade the performance, we can replace LibSci with ACML or MKL. On the other hand, although GROMACS uses FFTW functions, it is only compatible with FFTW3. As a result, we can build nine versions of GROMACS on Kraken (i.e., gromacs-gnu-libsci, gromacs-gnu-acml, gromacs-gnu-mkl, gromacs-intel-libsci, gromacs-intel-acml, gromacs-intel-mkl, gromacs-pgi-libsci, gromacs-pgi-acml, gromacs-mkl), as shown in Table 3.

The benchmark results shown in the two figures below indicate that GROMACS compiled by GNU or Intel compilers outperforms that compiled by PGI compiler by 10 percent or so, while the Intel versions are slightly faster than GNU versions. The latter is the default version on Kraken. For this particular application, the numerical library does not appear to have any apparent influence on application performance.

Table 8. Performance data of GROMACS-D.DPPC (unit: second).

	12-core	**24-core**	**48-core**	**96-core**	**192-core**	**384-core**	**768-core**
GNU-libsci	3003.08	1292.85	651.81	331.58	171.75	89.57	47.32
GNU-acml	3001.98	1293.35	648.82	330.36	171.79	89.01	45.49
GNU-mkl	3002.34	1289.56	650.21	332.63	171.76	88.90	45.26

Intel-libsci	2961.51	1267.52	637.60	323.83	176.01	87.50	45.23
Intel-acml	2959.81	1270.14	637.09	327.93	169.76	87.74	44.48
Intel-mkl	2961.12	1267.03	636.73	323.77	169.60	88.17	44.97
PGI-libsci	3267.51	1407.30	704.72	358.31	188.16	96.24	52.02
PGI-acml	3268.21	1405.02	704.99	358.31	190.41	96.57	51.90
PGI-mkl	3267.17	1409.91	705.62	359.50	190.71	96.87	52.38

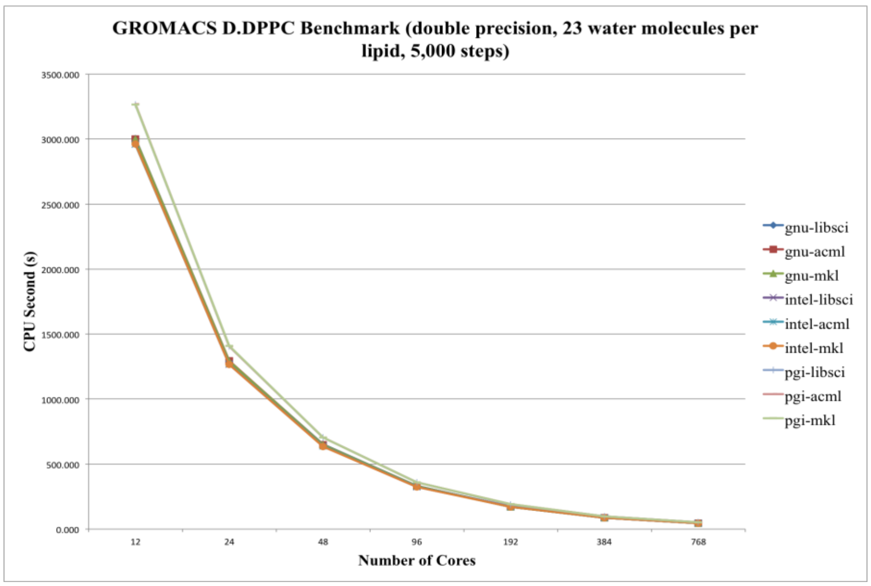


Figure 10.2-9. Performance data of GROMACS-D.DPPC.

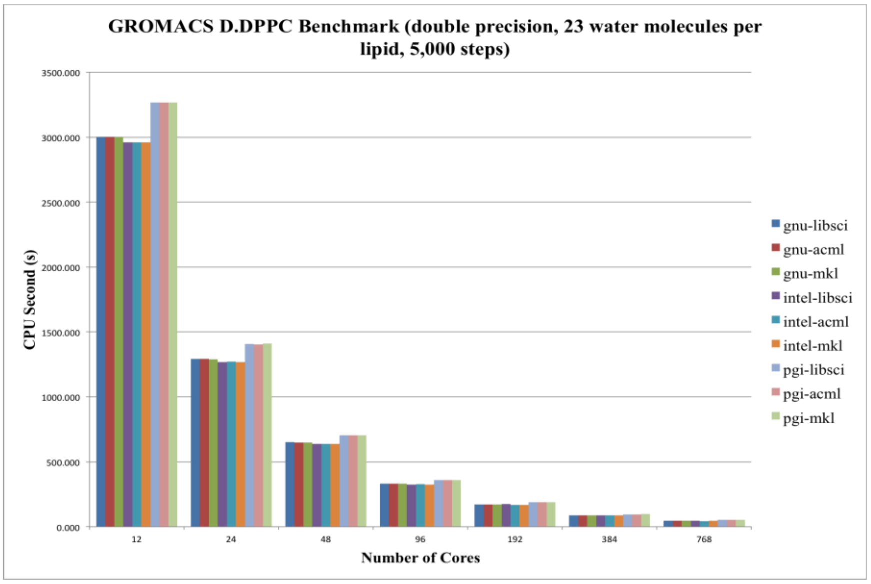


Figure 10.2-10. Performance data of GROMACS-D.DPPC.

10.2.2.4 CPMD

CPMD is a typical application that can be optimized by varying a number of configuration options: compiler, numerical library, and FFTW version. Theoretically, we are able to produce 18 versions of CPMD on Kraken. However, the latest source code version of CPMD is not compatible with the version of the GNU compiler on Kraken. Consequently, the GNU compiler does not work for this application in our study. We can then produce 12 versions of CPMD in total. Initially we ran the SI512 benchmark test for CPMD. It did not run when the number of nodes involved was one or two due to its memory-intensive nature. As a result, the C120 benchmark test was also adopted.

Table 9. Performance data of CPMD-SI512 (unit: second)

	48-core	**96-core**	**192-core**	**384-core**	**768-core**
Intel-libsci-fftw2	257.25	155.06	88.68	90.50	144.72
Intel-libsci-fftw3	249.26	163.64	89.93	109.64	100.85
Intel-acml-fftw2	236.24	124.74	67.40	69.24	38.00
Intel-acml-fftw3	228.87	118.58	66.12	40.10	34.41
Intel-mkl-fftw2	155.34	95.53	54.52	54.47	63.18
Intel-mkl-fftw3	152.21	89.94	53.98	49.43	51.71
PGI-libsci-fftw2	239.91	285.96	234.12	512.95	127.33
PGI-libsci-fftw3	231.98	289.82	226.53	143.74	132.31
PGI-acml-fftw2	235.96	290.20	204.43	130.77	167.86
PGI-acml-fftw3	230.73	285.73	193.29	129.62	149.68

PGI-mkl-fftw2	160.96	290.71	193.24	139.33	155.72
PGI-mkl-fftw3	157.28	288.34	182.21	172.41	165.06

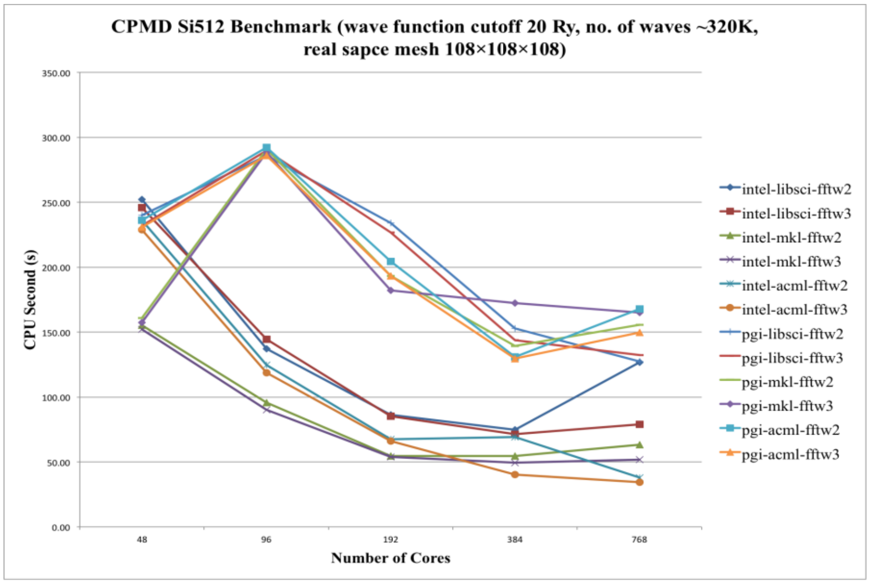


Figure 10.2-11. Performance data of CPMD-SI512.

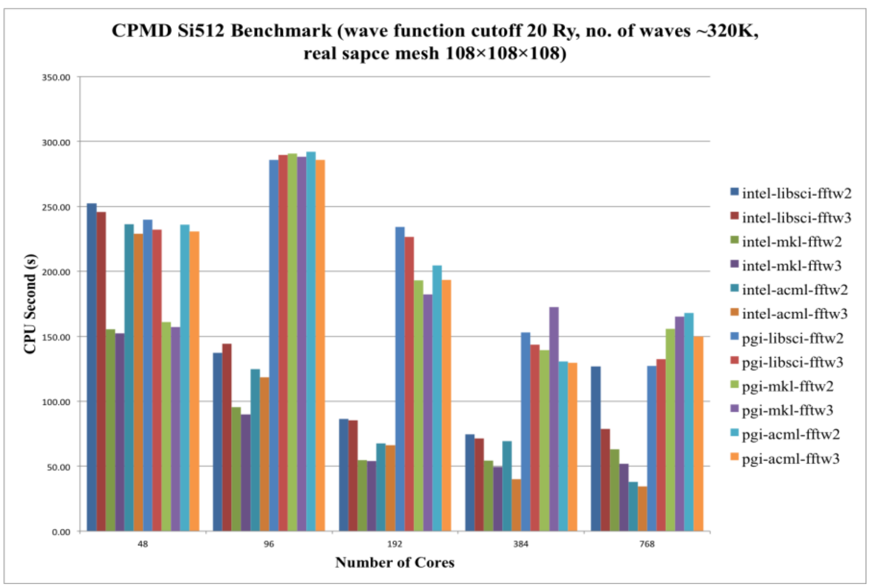


Figure 10.2-12. Performance data of CPMD-SI512.

From the performance results for CPMD-SI512, shown in Figures 10.2-7 and 10.2-8 above, it is obvious that the choice of compiler can make a substantial difference. *The Intel compiler is better in most cases. It can improve the speed up to 4 times* (e.g., intel-acml-fftw3 vs. pgi-acml-fftw3). For the PGI version of CPMD, the performance degrades significantly when the number of cores increases from 48 to 96. This is also true in some cases even for 192 cores. On the other hand, the right choice of FFTW version can benefit the performance to some extent. For CPMD, the numerical library does matter. For example, if built with the Intel compiler, the MKL library usually produces better performance. The FFTW3 version outperforms its FFTW2 counterpart in most cases. Also, it is striking to see that with 384 cores, intel-mkl-fftw3 is more than 10 times faster than pgi-libsci-fftw2 (the default version on Kraken). Finally, please note that for CPMD, a larger number of cores does not necessarily produce better performance.

Table 10. Performance data of CPMD-C120 (unit: second).

	12-core	24-core	48-core	96-core	192-core	384-core	768-core
Intel-libsci-fftw2	2429.96	1583.14	605.01	283.78	137.54	94.44	109.83
Intel-libsci-fftw3	2342.36	1187.47	487.14	306.64	126.43	82.04	75.41
Intel-acml-fftw2	2492.03	1280.99	825.91	277.79	134.56	84.44	165.56
Intel-acml-fftw3	2181.51	1167.62	556.35	258.16	122.54	74.09	158.31
Intel-mkl-fftw2	2353.55	1287.00	604.83	243.03	121.84	82.70	245.32
Intel-mkl-fftw3	2009.46	1272.34	512.59	586.94	135.60	81.51	184.11
pgi-libsci-fftw2	2492.03	1280.99	825.91	277.79	134.56	84.44	165.56
PGI-libsci-fftw3	2181.51	1167.62	556.35	258.16	122.54	74.09	158.31
PGI-acml-fftw2	2559.22	1267.94	672.51	291.67	160.00	91.04	96.01
PGI-acml-fftw3	2148.54	1139.67	673.84	286.98	152.62	80.44	136.20
PGI-mkl-fftw2	2389.11	1075.55	583.22	292.65	154.56	89.78	157.16
PGI-mkl-fftw3	2384.37	1054.99	598.94	295.88	168.19	100.78	102.42

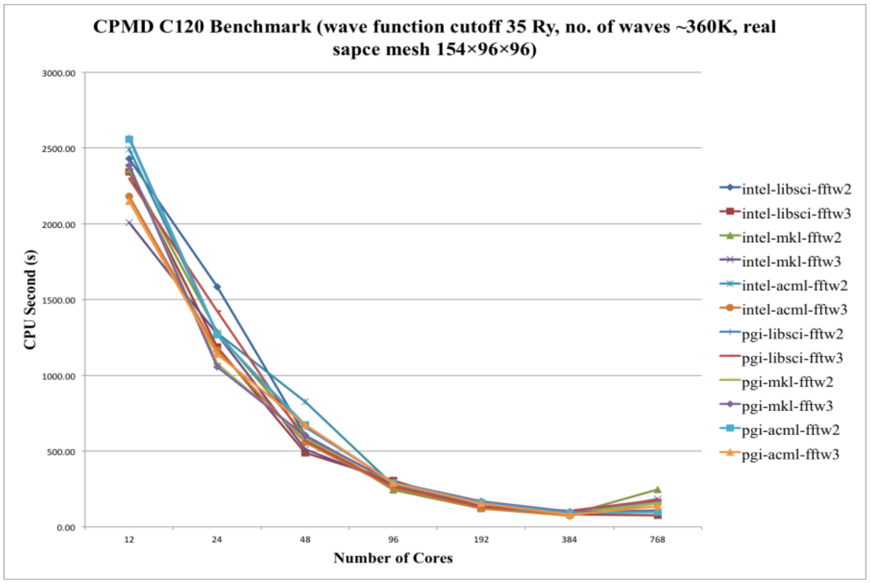


Figure 10.2-13. Performance data of CPMD-C120.

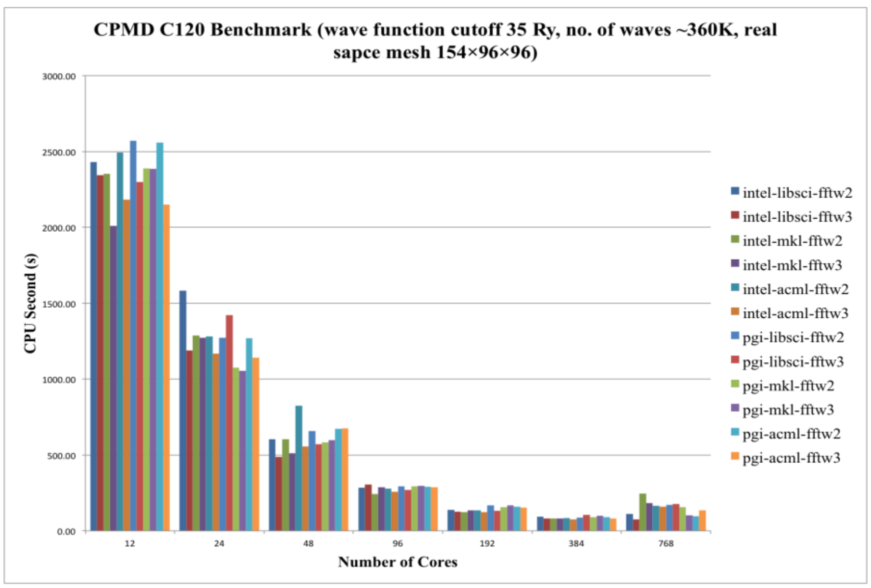


Figure 10.2-14. Performance data of CPMD-C120.

Similar to the CPMD-SI512 benchmark, the choice of compiler can make a big difference with the CPMD-C120 benchmark, as shown in the two figures above. However, the results are not consistent. Sometimes the Intel compiler is better, while in other cases the PGI compiler produces better results, depending upon the number of cores the application runs on. This benchmark also shows that the numerical library can influence the performance to some extent. Again, the choice of FFTW version is critical. With the same compiler and numerical library, FFTW3 outperforms FFTW2 significantly in most cases.

10.2.2.5 AMBER

AMBER uses BLAS/LAPACK functions so we have three options of numerical library. Although it needs to be linked with FFTW, only FFTW3 is compatible. Therefore, as shown in Table 6, we can produce nine versions of AMBER: amber-gnu-libsci, amber-gnu-acml, amber-gnu-mkl, amber-intel-libsci, amber-intel-acml, amber-intel-mkl, amber-pgi-libsci, amber-pgi-acml, amber-pgi-mkl. For some unknown reason, the Intel versions do not work properly on Kraken.

Table 11. Performance data of AMBER-JAC (unit: second)

	24-core	48-core	96-core	192-core	384-core	768-core
GNU-libsci	140.12	70.89	36.62	20.05	11.78	8.54
GNU-acml	139.93	70.99	36.67	19.95	12.95	8.59
GNU-mkl	139.92	70.87	36.89	19.78	12.32	10.96
PGI-libsci	107.21	55.04	29.18	16.65	10.92	8.79
PGI-acml	107.29	55.06	28.96	16.73	10.52	8.53
PGI-mkl	107.26	55.06	28.94	16.82	10.84	9.77

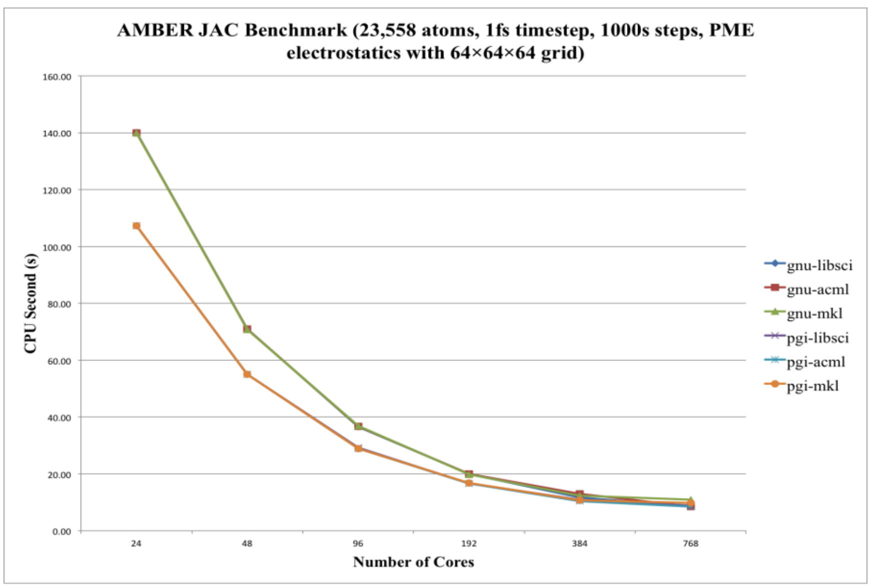


Figure 10.2-15. Performance data of AMBER-JAC.

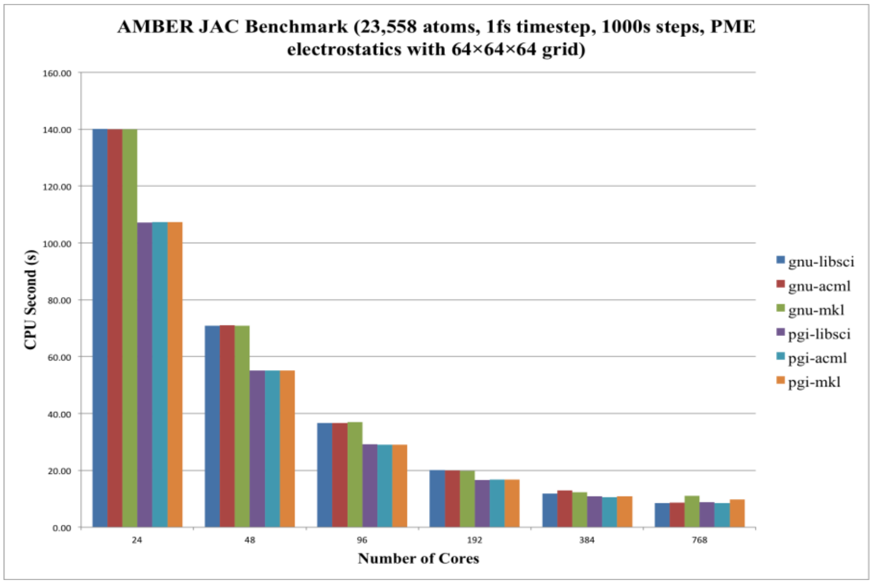


Figure 10.2-16. Performance data of AMBER-JAC.

As shown in the two figures above, AMBER built by the PGI compiler appears to run much faster than that built by the GNU compiler. Unlike CPMD, the selection of numerical library does not make any difference, except that the MKL versions are slower than their LibSci and ACML counterparts when running on 768 cores.

10.2.3. PEAK Conclusions

Through this study of the configuration of scientific applications, we learned that:

1. Application performance usually varies to a certain extent by selecting different compilers. Sometimes the right choice provides substantial improvement (as much as a factor of 4).
2. Selection of numerical libraries and FFTW version can influence the execution speed in some cases. CPMD represents a typical example in this study.
3. For HPC users, the optimized configuration of an application is not always the same. The best choice can vary based on the number of cores an application runs on.

An optimal application configuration is critical to achieve an efficient usage of HPC resources by end users, and PEAK can be used to provide the optimized solution for each application.

10.2.4. Future Work on Peak

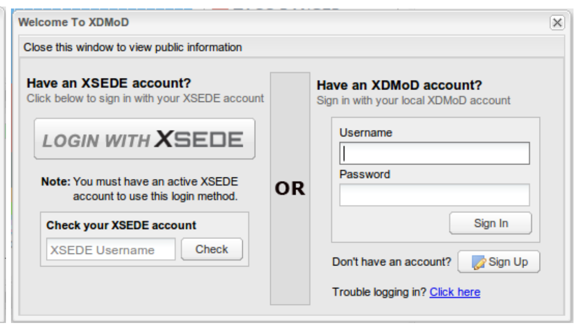
In the next phase, we are planning to port our work to other XSEDE platforms and integrate PEAK into the XDMOD framework. We have all the configuration, job submission, and result analysis scripts for each application ready. Slight modifications are expected to make them run successfully on other platforms. Another application of this study is to generate service units (SUs) conversion comparison between XSEDE supercomputers specific for each application.

10.3 University of Michigan Sub-contract: Usability assessment report:

At the end of Q3 the team at the University of Michigan School of Information (UMSI) delivered a usability report on the XDMoD interface. The report highlighted issues exposed by observing and interviewing potential and actual users of XSEDE spanning a range of novice to expert opinions. A number of issues concerned information overload, such as the cluttered XDMoD login window, and these were addressed in Q4. For example, in the image below, the window on the left shows the original implementation of XDMOD. The revised version, on the right, incorporates feedback from the UMSI report and has 20% less text, reserves color fonts only for important user actions (such as seeking help), and emphasizes the distinction between the XSEDE and XDMoD accounts.

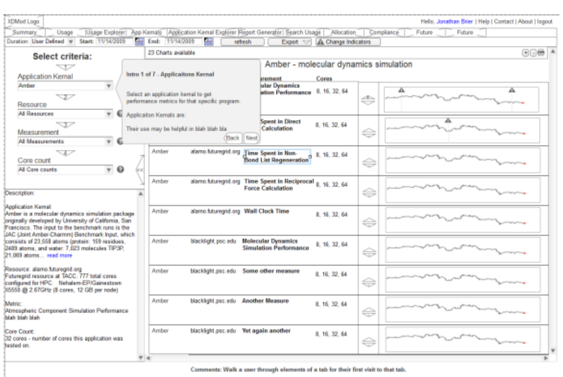
Previous login window

Revised login window

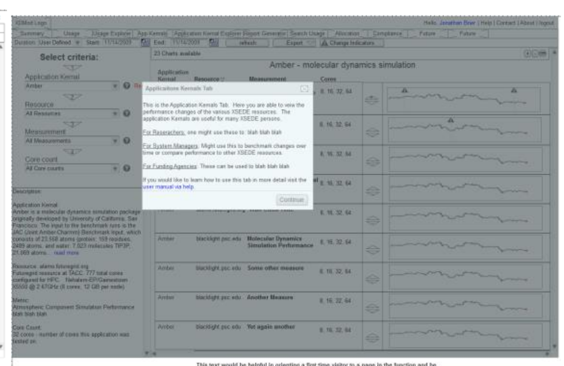


Other changes followed from recommendations to address usability for new users. For example, in the image on the left below, the pop up tutorial alerts users to a new feature. In the image on the right, instructions are overlaid where a user is attempting to perform a new action. Both of these improvements are designed to give the user quick, easy to understand directions on how to use complex XDMoD features.

Pop up tutorial

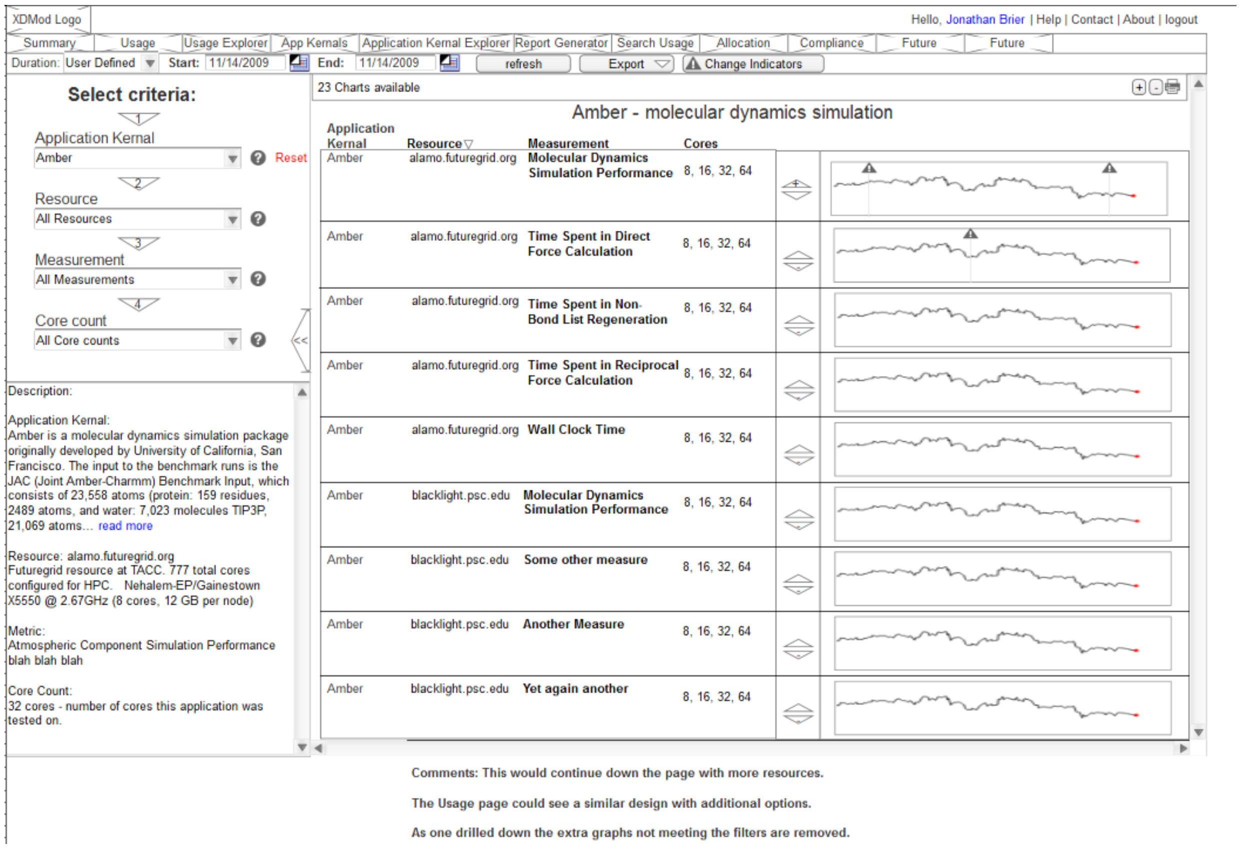


Overlay instructions

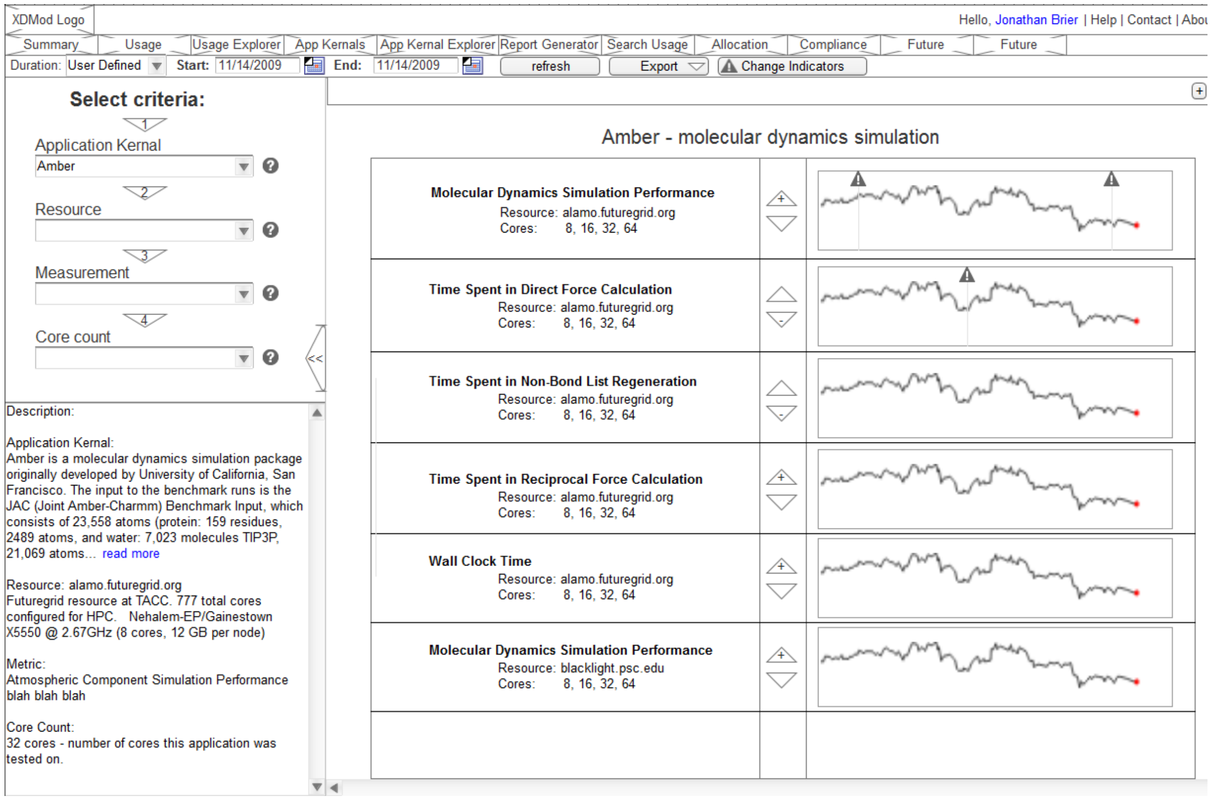


Finally, additional changes reflected suggestions for more design consistency. For instance, the images below show the evolution of the App Kernel page from the original approach Ap Kernel Concept 1 (upper figure) to the revised approach Ap Kernel Concept 2 (lower figure) re-designed to better match the Usage Explorer page.

App Kernel Concept 1



App Kernel Concept 2



Other usability issues identified in the UMSI report ran deeper and may require rethinking of design function to accommodate user needs. For instance, users are confused about why they must have separate XSEDE and XDMoD accounts. A single account system for all of XSEDE and related resources would simplify permissions and reduce complexity for users. Permissions could be enabled or disabled based on allocation and resource access.

The principal focus of the UMSI team during Q4 was the design, deployment and analysis of an XDMoD user survey. Targeted at a large, random, and representative sample of XSEDE users, the goal of the survey is to evaluate XDMoD from the perspective of the broad XSEDE community. By contrast, prior usability work by the UMSI team has focused only on local XSEDE users. The survey instrument covers: heat map tracking of user clicks (e.g., percentage of respondents who correctly identify the button to perform a targeted function); demographics (e.g., gender, role, age); attitudinal measures (e.g., satisfaction with XDMoD); behavioral measures (e.g., recency of XSEDE use); and free text responses (e.g., additional thoughts or opinions). The instrument was improved through iterative rounds of testing.

Originally scheduled for completion during Q4, the survey effort was delayed due to complications associated with a novel pre-incentive design (i.e., the small tokens or cash gifts given to respondents to encourage completion of the survey). Ultimately, the UMSI team abandoned the novel pre-incentive scheme and the survey was deployed in December, about two months later than scheduled. The delay did not impair response: 30% of those sampled completed a survey (typical response rates for online surveys are between 20 to 25%). The main consequence of the delay was that the analysis phase was pushed to Q1 of 2013. While exhaustive analysis of the survey results are still underway, preliminary findings are promising. For example, the heat map data indicate that the orientation instructions added to the blank Report Generator and App Kernels Explorer tabs help users in performing the correct actions.

10.4 Indiana University Sub-contract: Progress report

We collaborated with the FutureGrid team in the development of a metric report generation system. We created an online and offline prototype reporting system that is significantly different in scope and metrics from the available XSEDE system. The differences include: a) it is explicitly targeted for Cloud IaaS frameworks and includes metrics for VMs.

We have continued working on our scholar publication identification framework for XSEDE users. We explored the possibility of obtaining publication data from a Google Scholar user profile. We were able to parse the profile page to get the list of publications and the metrics computed by Google if the user's profile is public and we know the Google scholar user id. This has been put into the prototype framework we have been working on. In addition, we have been working on integrating additional data sources into the prototype. This includes a) information from the NSF award search library, and b) information from the processed POPS publication data we obtained from XSEDE. We were able to output a list of publications from these two sources for specific author names. We are planning to correlate this information with other data sources like the XDCDB user data and POPS grant data.

Outlook: So far we have concentrated on the data acquiring process from various sources. For each of the sources, we would like to setup an intermediate database so the preprocessed results could be stored and updates can be integrated periodically. This database meshup will than serve as the information source from where we expose the data via web services or directly input the data to XDMOD.

10.5 XDMoD Usage:

XDMoD 2.5 (https://xdmod.ccr.buffalo.edu), was released just before SC12. XDMoD usage during the present reporting period is shown in Figure 10.5-1. Figure 10.5-2 shows the growth in XDMoD usage over the past two years. While the usage is substantially increased over the last quarter, we anticipate increased usage in the future as more users become aware of its availability and capability.

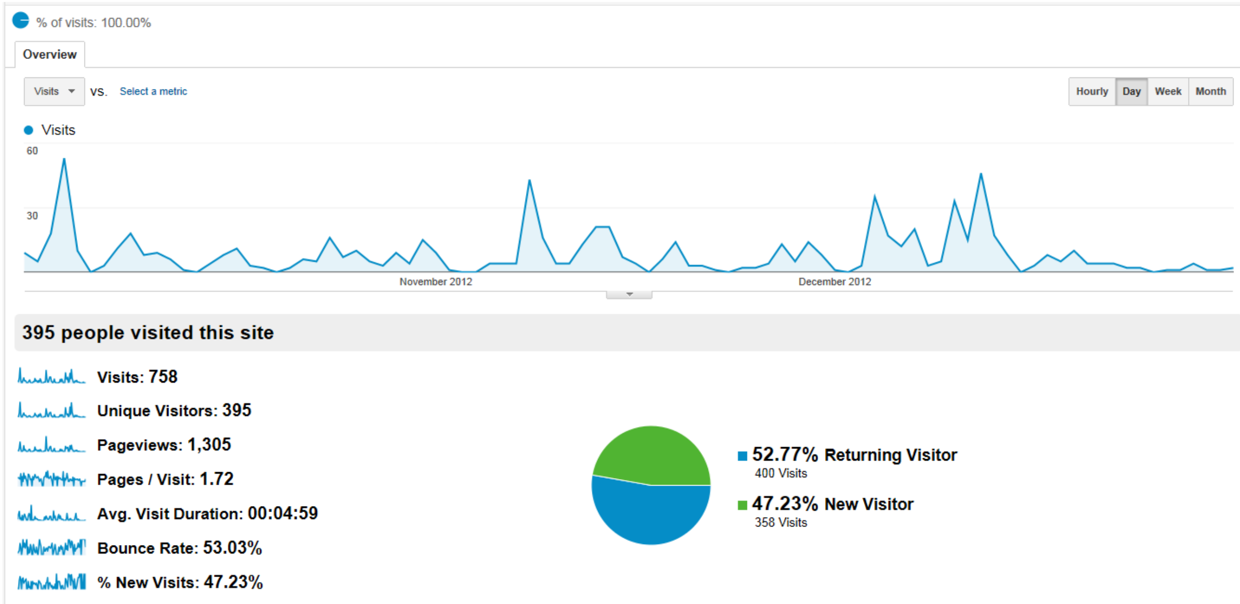


Figure 10.5-1. Google analytics overview of XDMoD usage for October 1, 2012 to December 31, 2012.

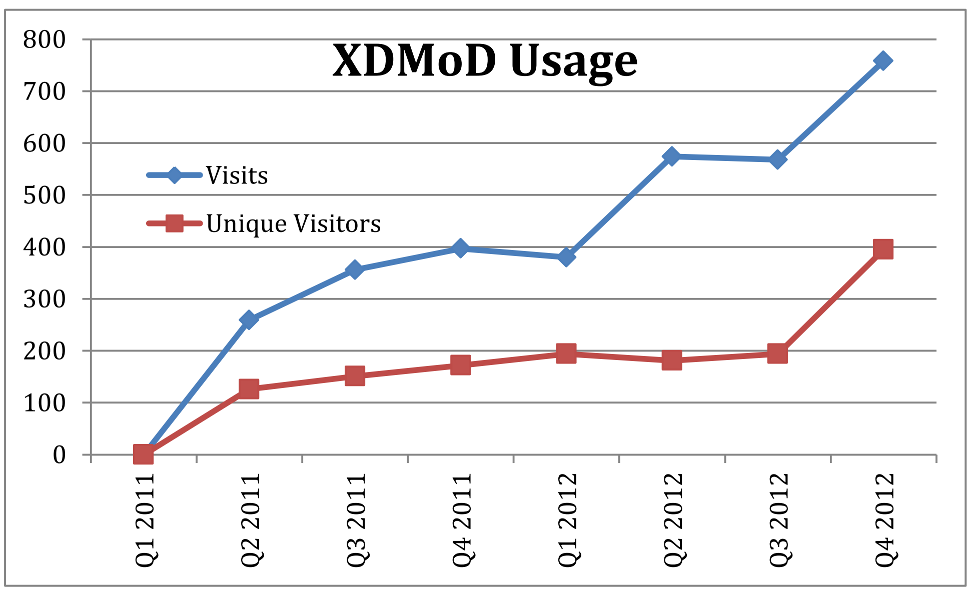


Figure 10.5-2. Growth in XDMoD usage for the past 2 years.

10.6 Coordination with External Projects and Agencies

TAS has an active role in the effort to upgrade the POPS allocation process and database. Steve Gallo, who oversees the XDMoD software development for TAS, sits on the XSEDE-wide committee that is tasked with developing the POPS 2.0 framework. This will help ensure that the new POPS database collects information required for the desired level of reporting and better interoperates with XDMoD and therefore will allow XDMoD to more readily display metrics related to grants, allocations, field of science, and publications.

TAS has been in an active collaboration with XSEDE and Open Science Grid (OSG) to develop a conceptual design to merge the features of OSG's accounting system (Gratia) with XDMoD to develop a unified usage and auditing service for cyberinfrastructure providers.

10.7 Meetings, Events Publications and Presentations

TAS team members attended SC12 in Salt Lake City (November 2012).

TAS SC12 Attendees included: Dr. Thomas Furlani, Dr. Matthew Jones, Mr. Steven Gallo, Mr. Ryan Gentner, Mr. Amin Ghadersohi, Mr. Jeffrey Palmer, Dr. Charng-Da Lu, Dr. Robert L. DeLeon, Dr. Gregor von Laszewski (IU), and Dr. Fugang Wang (IU).

SC12 Birds-of-a-feather presentation made on Nov 14, 2012:

XSEDE Metrics on Demand (XDMoD) Technology Auditing Framework;

Presented by: Thomas R. Furlani, Matthew D. Jones and Steven M. Gallo

ABSTRACT:
XDMoD (XSEDE Metrics on Demand) is an open-source tool designed to audit and facilitate the utilization of XSEDE cyberinfrastructure, providing a wide range of metrics on XSEDE resources and services. Currently supported metrics include allocations and computing utilization, allowing a comprehensive view of both current and historical utilization, and scientific/engineering application profiling (via application kernels) for quality of service. XDMoD (https://xdmod.ccr.buffalo.edu) uses a role-based scheme to tailor the presentation of information to the public, individual users, principal investigators, service providers, campus champions, and program managers. At this BOF the current state of XDMoD will be demonstrated and discussed.

Mr. Ryan Gentner and Mr. Amin Ghadersohi attended a conference on web-based programming: "The Rich Web Experience 2012", November 27 - 30, 2012 in Fort Lauderdale, FL

11 ExTENCI

11.1 Overview

The goal of The Extending Science Through Enhanced National Cyberinfrastructure (ExTENCI) Project is to develop and provide production quality enhancements to the national cyberinfrastructure that will enable specific science applications to more easily use both OSG and XSEDE or broaden access to a capability to both XSEDE and OSG users.

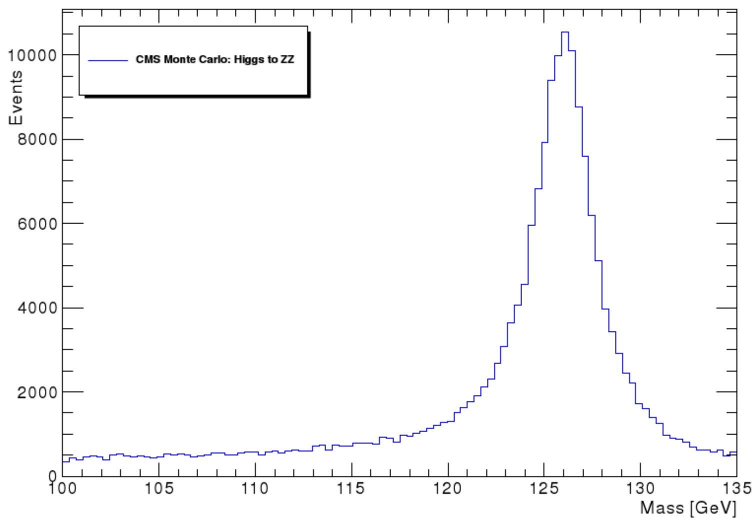
The ExTENCI Project is a joint Open Science Grid (OSG) and TeraGrid/XSEDE project, funded by OCI. The PIs are Paul Avery (U. Florida) and Ralph Roskies (PSC). The planned two-year project began in August 2010 and has received a no-cost extension through July 2013.

Overall, the project has completed 99 of the 123 total deliverables, counting new deliverables defined at the end of year 2. ExTENCI has four primary areas of work, each of which is discussed sections below.

11.1.1 ExTENCI – Distributed File System (Lustre-WAN)

This quarter, a major stability problem with the Lustre client was resolved by Whamcloud which allowed performance and production testing to continue. Kerberos-Lustre, needed to provide authentication in a university environment that is based on Kerberos, is now stable. Work to interface with XRootD storage systems and Global Federated Filesystems was completed and tested. Progress in these areas enabled FIU to run Higgs boson simulations using data from UF via Lustre, a major goal of the DFS team.

- CMSSW muon analysis has been running in **production-mode** on FIU's **200-core (25 nodes**) cluster using the ***hybrid kerberos-lustre-XRootD*** setup with no problems.
    - FIU DGT client is exporting lustre to 25 compute nodes via XRootD
    - Stability has been achieved for the kerberized lustre filesystem
    - Production-level tests with 200 CMSSW_3_9_9 MuonAnalysis reconstruction jobs reading input from /extenci, were submitted by Condor to FIU's 25 compute nodes. All the CMSSW jobs finished without any error.
- JIRA whamcloud updated their Lustre release with a generally available patch that has addressed our client stability problems.
- PSC Client
    - Installed full Globus/Grid software with kerberos keys and certificates used by XSEDE
    - Installed/enabled Global Federated Filesystem (GFFS) container/client
- Writing from computation nodes via XRootD to /extenci is now possible via a direct unix path. The XRootDfs package based on fuse allowed POSIX-compliant-operations on compute nodes on /extenci done by normal unix path instead of special root://URL. This is a significant achievement allowing general applications without XRootD plug-in to have simple access to /extenci lustre fs
- We ran simplified version of Higgs histogram AOD format reconstruction of Higgs decaying to two Z bosons and then decaying to four charged leptons using Monte-Carlo simulation data borrowed from UF CMS Tier2 data center. The test has been repeated several times for different number of events and we reproduce the Higgs peak ~126GeV as shown in diagram. The test is CPU intensive and the processing time per event was constant for 1000 to 100K events.



- Results of Higgs Boson task were presented at SC2012
- Verified that Lustre throughput on the Higgs reconstruction jobs scales linearly up to the throughput of the network

11.1.2 ExTENCI – Virtual Machines

One of the deliverables of the VM team was to develop a Dashboard that enables a user to obtain and configure virtual machines using a graphical user interface. This was done early in 2012 and is now FutureGrid is interested in making the Dashboard available to it users.

- Supplied a non-HUBzero version of the Dashboard to FutureGrid.
- Parallelized a simulation in material science using the Chemistry molecular dynamics application Gromacs and built a control workflow to do the simulations using Hadoop.

11.1.3 ExTENCI – Workflow & Client Tools

The WCT team has been working on interfacing Swift to a broader number of execution environments. This quarter, the team prepared a new software release containing cloud support, improved error reporting, added interface to new job schedulers, and improved support of MPI applications. The team continued to work with scientists doing protein research and began work with animal biology bioinformatics, the latest in a series of applications using the new capabilities of Swift.

- Posted a Swift 0.92RC2 release and continue QA and improvements on it.
- Integrated and tested with the latest Nimbus Phantom tools to update Swift cloud support.
- Made significant improvements to Swift error reporting and process tracebacks
- Added support for the LSF and SLURM schedulers
- Enhanced support for flexible Condor configurations
- Added ability to reach remote sites via command-line ssh for BOSCO-like capabilities.
- Improved support for MPI applications
- Integrated revised protein folding application code
- Started work on new animal biology bioinformatics application “EpiSnp” for a U. of Minnesota and U. of Chicago collaboration. Integrated this into the GPSI web portal.

- Hocky produced a new science paper posted on ArXiV: http://arxiv.org/abs/1211.0033 that was enabled by ExTENCI work

11.1.4 ExTENCI – Job Submission Paradigms

The JSP team continues to enhance and add plug-in adaptors on SAGA to enable science jobs and data to be distributed to both XSEDE and OSG.

- Updated Condor plug-in for SAGA-Python (Bliss) -- both XSEDE and OSG resources can now be accessed through the same SAGA codebase
- Started work on iRODS plug-in for SAGA-Python in order to support data-intensive use-cases on OSG
- Restarted efforts with Science Gateway Developer to integrate SAGA into the gateway

12 XD Service Provider Reports

2012 Q4: October 1, 2012, through December 31, 2012

XD Service Provider Forum Leadership

Carol Song, Chair	Purdue University
David Y. Hancock, Vice Chair	Indiana University

XD Service Provider Principal Investigators

Sean Ahern	U Tennessee – National Institute for Computational Science
Jay Boisseau	U Texas - Texas Advanced Computing Center
Geoffrey Fox	Indiana University
Kelly Gaither	U Texas - Texas Advanced Computing Center
William T.C. Kramer	UIUC/NCSA (Blue Waters)
Michael Levine	Pittsburgh Supercomputing Center
Miron Livny	U Wisconsin-Madison
Richard Loft	National Center for Atmospheric Research
Richard Moore	U California San Diego - San Diego Supercomputer Center
Michael Norman	U California San Diego - San Diego Supercomputer Center
Manish Parashar	Rutgers University
Gregory D. Peterson	U Tennessee – National Institute for Computational Science
Carol Song	Purdue University
Craig Stewart	Indiana University
John Towns	U Illinois - National Center for Supercomputing
Jeffrey Vetter	Georgia Institute of Technology

12.1 Overview

The XD Service Provider (SP) Forum is the representative body of federated providers of leading-edge computational, storage and visualization resources, software and associated services to the open science community. In partnership with the XSEDE project, the SPs have delivered more than 803 million service units (SUs) collectively to the XSEDE user community in this quarter, supporting 2331 users from 334 institutions. Below is a summary of the SP Forum's activities in this quarter.

Membership:

The SP Forum (SPF) completed the review and approval of all the pending membership applications from the interim forum members. The complete list of current forum members is available at: https://www.xsede.org/web/sp-forum/spf-membership/-/wikid/LU1q/Public/Spf-members.

In December, the SP Forum accepted Blue Waters SP as a new member of the SP Forum. The Blue Waters project has and continues to reach the XSEDE community in multiple ways including jointly with XSEDE hosting summer schools, training, workshops, as well as training and education offerings to the education community K-12 – postgraduate education. These efforts help to develop a foundation in HPC thereby benefiting the greater community of HPC users. The Blue Waters SP is currently admitted to the SP Forum as a Level 3 SP until such time when Blue Waters joins the XSEDE Federation and its Level is determined.

Storage Allocations Implementation:

The SP forum has worked with the XSEDE project to define and formalize the storage allocations policy. The Forum has approved the final version of the XSEDE storage allocations policy. The four SPs who will provide storage resources to be allocated under the new storage allocation policy have agreed to a set of thresholds, including the maximum storage space with SP approval and length of retention period after project expires. The XSEDE project will provide timeline and specifics of the implementation to the SPs to ensure readiness for the March 2013 XRAC allocation.

Response to NSF Reorganization:

In response to the recent NSF reorganization in which the Office of Cyberinfrastructure (OCI) is being merged into the CISE directorate, the SPF delivered a letter to the NSF Advisory Committee for Cyberinfrastructure outlining the concerns and recommendations of its members in October.

Additional Information:

The SPF conducts its business and coordination through regular conference calls on Tuesdays at 11am Eastern Time. Victor Hazlewood has been named in the role of the XSEDE SP coordinator and has a monthly presentation to the SP Forum to provide updates on XSEDE operations. The Forum Chair and Vice Chair participated in the XSEDE quarterly meeting in December, as well as the regularly Senior Management Team calls.

13 XSEDE Quarterly Report: FutureGrid Service Provider (October 1, 2012 – December 31, 2012)

13.1 Executive Summary

- ScaleMP completed certification of their software on the new Intel Sandy Bridge cluster. ICC will ship the 16 servers to Indiana and implementation of the new FutureGrid ScaleMP cluster will commence in January.
- FutureGrid demonstrated at SC'12
- Planning underway for the Spring 2013 FutureGrid User Survey
- Upgraded the Cray XT5m (*xray*) to CLE 3.1UP03A with SLES-11 and Cluster Compatibility mode.

13.1.1 Resource Description

FG Hardware Systems

Name	Site	System type	# Nodes	# CPUs	# Cores	TFLOPS	Total RAM (GB)	Storage (TB)
		Operational						
india	IU	IBM iDataPlex	128	256	1024	11	3072	335
hotel	UC	IBM iDataPlex	84	168	672	7	2016	120
sierra	SDSC	IBM iDataPlex	84	168	672	7	2688	96
foxtrot	UF	IBM iDataPlex	32	64	256	3	768	0
alamo	TACC	Dell PowerEdge	96	192	768	8	1152	30
xray	IU	Cray XT5m	1	168	672	6	1344	335
bravo	IU	Large Disk / Large Memory	16	32	128	1.5	3072	192
delta	IU	Large Disk / Large Memory With Tesla GPUs	16	32 CPU 32 GPU	192 14336	9	1536	192
Total					**4384**			
		Other						
lima	SDSC	SSD	8	16	128	1.3	512	3.8 (SSD)
		Implementation						
echo	IU	Large Disk / Large Memory (for ScaleMP software)	16	32	192	2	6144	192

FG Storage Systems

System Type	Capacity (TB)	File System	Site
Xanadu 360	180	NFS	IU
DDN 6620	120	GPFS	UC
SunFire x4170	96	ZFS	SDSC
Dell MD3000	30	NFS	TACC
IBM dx360 M3	24	NFS	UF

13.2 Science Highlights

GridProphet, A workflow execution time prediction system for the Grid

Thomas Fahringer
Institute for Computer Science
University of Innsbruck

Abstract

Workflow applications have provided a dynamic and heterogeneous paradigm for execution of computationally large experiments on the Grid and have greatly increased the pace of scientific work. Through their distributed task based execution mechanism, they have eliminated the need for resource homogeneity. A Grid workflow application represents a collection of computational tasks (activities) interconnected in a directed graph through control and data flow dependencies that are suitable for execution on the Grid. The complexity of the workflows has increased over the years with the increasing complexity of scientific applications. A common measure for the performance of scientific workflow applications is the total execution time needed to finish the entire workflow. The objective of this project is to develop a grid performance prediction system, which can estimate the execution time of individual workflow tasks, single-entry-single-exit sub-workflows (e.g. loops), and entire workflows for scientific applications such that the prediction technology can be used to rank different workflow transformations or workflow versions with respect to their execution time behavior. The proposed system can be used for optimization of workflow applications, thus enabling scientists to better utilize computing resources and reach their scientific results in shorter time.

Intellectual Merit

The intellectual merits of this research lie in the following contributions to the fields of scientific workflows and Grid computing. The development of a prediction model based on advanced statistical techniques and machine learning methods to support :

1. The modeling of execution behavior of highly distributed grid workflows,

2. The development of an execution trace collection and performance prediction system for Grid workflow execution environments.

3. Querying and utilization of historical trace data on-the-fly for accurate prediction of grid workflow execution time using machine learning based prediction system.

Broader Impacts

The success of this project will provide a general-purpose tool for execution time prediction for Grid workflow and will help the Grid users for efficient grid resource utilization. The tool would be customizable for use with other Grid workflow systems as well.

Use of FutureGrid

The primary use of the FutureGrid infrastructure is to execute large number of Grid workflow applications and collect the execution trace for these execution to be fed to the machine learning system for training the machine learning.

Results

Project brief:
This project was initiated as part of a larger project titled "A provenance and performance prediction system for Grid systems". The objective of the main project is to develop a grid performance prediction system, which can estimate the execution time of individual workflow tasks, single-entry-single-exit sub-workflows (e.g. loops), and entire workflows for scientific applications such that the prediction technology can be used to rank different workflow transformations or workflow versions with respect to their execution time behavior. The proposed system can be used for optimization of workflow applications, thus enabling scientists to better utilize computing resources and reach their scientific results in shorter time. The objective of the utilization of Future Grid resources was to collect trace data for training the machine learning systems. The data collected using the Future Grid resources is used along with the data traces collected in the Austrian Grid and the Grid5000.

Experimental Setup:

Grid-Appliance provided by Future Grid portal is used in varying configuration to setup the Virtual Grid required to serve the project objective. Based on the project requirements trace collection was to be performed for the following applications:

•MeteoAG (Meteorology Domain)

•Wien2K (Material Science Domain)

•InvMod (Alpin River Modeling)

The goal was to record trace collection data for atleast 5000 workflow runs in total with varying background load and dynamic distribution of tasks on different sites in the virtual Grid. For this purpose the Grid-Appliance was customized in different aspects. Additional software packages were added required for the execution of the workflow execution system (ASKALON) and the workflows themselves. A database server was installed to collect the trace data during the experiments.

Trace Data:

A set of key features having noticeable importance during the execution of these workflows on the Grid infrastructure was identified. These selected features covered most of the factors associated to Grid workflow execution such as input to the application workflow, size of the input data, size of application executables, Network associated features like available bandwidth, bandwidth background load, time required to transfer the application data across computer nodes. Moreover both the dynamic and static environment associated parameters are also collected which include the information about the machine architecture, compute power, cache memory and disk space etc. A total number of 65 parameters are selected for use to get accurate predictions and for a rich machine learning based training of the prediction model.

Optimization of the Feature Vectors:

For use with the machine learning system the main feature vector is shortlisted to select a small number of parameters, so that the machine learning process can be carried out swiftly and accurately. Having a large number of input parameters results in very long training times and also introduces lots of noise in the data. We recorded a large number of run-time parameters so as not to miss any important feature. But for the training of the model we needed to optimize the feature space so that the problems associated with the noise and long training durations can be avoided. Principal component analysis and Principal Feature selection algorithms are used for optimization of the feature space and an optimized feature vector is generated that have maximum influence on the execution of the tasks in distributed environments.

Utilization of Trace Data:

A neural network based machine learning system known as Multilayer Perceptron (MLP) is used. MLP is a Feedforward neural network system for training machine learning models and is used for pattern matching in non linear problem spaces. It maps the sets of inputs presented at the input layers of the network to outputs at the output layer. In contrast to the traditional neural networks MLP may have one or more hidden layers. An activation function determines the threshold value of the network at each node which acts a neuron for the neural network.

For our experiments the trace data collected from the Future Grid infrastructure was used along-with the data collected from other Grid infrastructures like that of Austrian Grid and the Grid5000. The training results presented herewith are therefore not specific to Future Grid only.

Performance Predication Results:

Based on our experiments and the machine learning system described above the following activity level predictions accuracy has been achieved.

Workflow: Wien2k

Total successful runs: 700

One activity maximum prediction accuracy: 65.70%

Two activities maximum prediction accuracy: 52.70%

Activity	Cluster	Prediction Accuracy
LAPW1	1	65.70%
LAPW1	2	63.00%
LAPW2	1	64.00%
LAPW2	2	60.00%
LAPW1,LAPW2	1	58.00%
LAPW1,LAPW2	2	56.00%
LAPW1,LAPW2	1	54.00%
LAPW1,LAPW2	2	52.00%

Single workflow prediction accuracy

The results presented above are quite promising for an initial investigation and therefore we are quite eager to continue this research to get even better results. Experimental workflow runs are in progress using the Future Grid resources to have more trace data for improved performance prediction accuracy.

Privacy preserving gene read mapping using hybrid cloud

Fusheng Wang
Center for Comprehensive Informatics
Emory University

Abstract

Study the possibility of doing reads mapping using hybrid cloud, in order to utilize public computing resources while preserving the data privacy.

Intellectual Merit

This research if of high demand in the area of bioinformatics as more and data are generated everyday but lack of computing resources to process them.

Broader Impacts

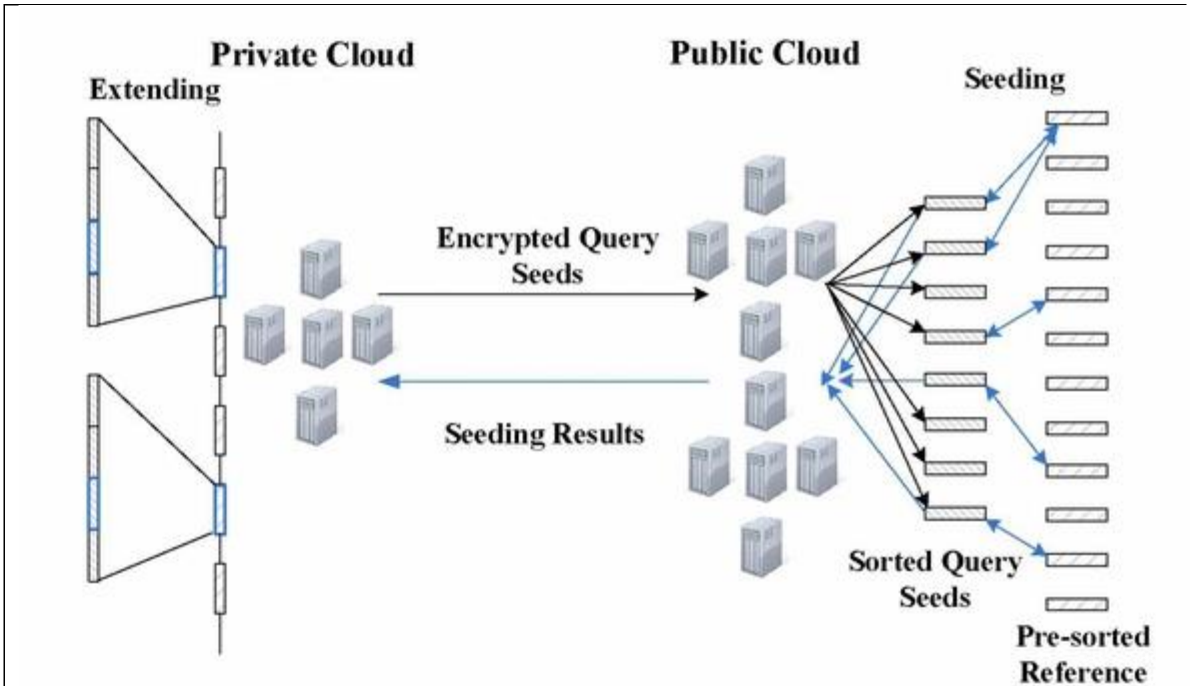
The research may increase data processing speed in the area of bioinformatics and thus replace current read mapping tools

Use of FutureGrid

Study privacy preserving computing using Hadoop as platform.

Results

One of the most important analyses on human DNA sequences is read mapping, which aligns a large number of short DNA sequences (called reads) produced by sequencers to a reference human genome. The analysis involves intensive computation (calculating edit distances over millions upon billions of sequences) and therefore needs to be outsourced to low-cost commercial clouds. This asks for scalable privacy-preserving techniques to protect the sensitive information sequencing reads contain. Such a demand cannot be met by the existing techniques, which are either too heavyweight to sustain data-intensive computations or vulnerable to re-identification attacks. Our research, however, shows that simple solutions can be found by leveraging the special features of the mapping task, which only cares about small edit distances, and those of the cloud platform, which is designed to perform a large amount of simple, parallelizable computation. We implemented and evaluated such new techniques on a hybrid cloud platforms built on FutureGrid. In our experiments, we utilized specially-designed techniques based on the classic “seed-and-extend” method to achieve secure and scalable read mapping. The high-level design of our techniques is illustrated in the following figure: the public cloud on FutureGrid is delegated the computation over encrypted read datasets, while the private cloud directly works on the data. Our idea is to let the private cloud undertake a small amount of the workload to reduce the complexity of the computation that needs to be performed on the encrypted data, while still having the public cloud shoulder the major portion of a mapping task.



We constructed our hybrid environment over FutureGrid in the following two modes:

1. Virtual mode:

We used 20 nodes on FutureGrid as the public cloud and 1 node as the private cloud.

2. Real mode:

We used nodes on FutureGrid as the public cloud and the computing system within the School of Informatics and Computing as the private cloud. In order to get access to the all the nodes on public cloud, we copied a public SSH key shared by all the private cloud nodes to the authorized_keys files on each public cloud node.

Our experiments demonstrate that our techniques are both secure and scalable. We successfully mapped 10 million real human microbiome reads to the largest human chromosome over this hybrid cloud. The public cloud took about 15 minutes to do the seeding and the private cloud spent about 20 minutes on the extension. Over 96% of computation was securely outsourced to the public cloud.

Evaluation of using XD TAS (Technology Auditing Service) in FutureGrid

Charng-Da Lu
Center for Computational Research
SUNY Buffalo

Abstract

This project will **explore how to utilize the XD TAS (Technology Auditing Service) framework as part of FG and identify if** modifications to TAS need to be made in order to fulfill the needs of FutureGrid.

Intellectual Merit--

Such a system is not available at this time in TG nor in other projects. There are only indifidually managed log files in the various cloud environments. Furthermore, we will help with the integration of auditing mechanisms into the HPC side of FG.

Broader Impacts

Users of FG will be able to visualize a lot of data related to usage of hardware and services. This data can be exposed based on role based access control. We will be working with the FG team to identify the security implications for authentication and authorization.

Use of FutureGrid

The use of FG is twofold: a) We will be exploring the use of TAS processes and technologies as part of FG. b) We will also work with the FG group to explore the use of TAS in cloud platforms.

Results

We have been running application kernels on FG systems for the past two years and we have collected their performance data, which can be viewed at XDMoD website (http://xdmod.ccr.buffalo.edu). We plan to continue running (and expanding) our set of application kernels and analyze the cause of performance fluctuations.

13.3 User-facing Activities

13.3.1 System Activities

13.3.1.1 Hardware

- IU iDataPlex ("*india*"). Upgraded all compute nodes with 3TB drives local storage (~2TB available to users as scratch space).
- IU Cray ("*xray*"). Upgraded to CLE 3.1UP03A with SLES-11 and Cluster Compatibility mode. Also upgraded the PGI and Cray compilers.
- IU HP ("*bravo*"). For this quarter 8 nodes dedicated to Dr. Martin Swany's InfiniBand research.
- IU GPU ("*delta*"). For this quarter 4 nodes dedicated to Karissa McKelvey's research efforts
- SDSC iDataPlex ("*sierra*"). Configured the storage on *sierra* to allow for mounts from the *lima* nodes so home directories and /N/soft can be leveraged from *sierra*. Upgraded Nimbus to 2.10.
- SDSC Aeon (*"lima"*). Working with users from University of Binghamton for early access and experimentation.
- UC iDataPlex ("*hotel*"). Implemented major disk reorganization to support higher Nimbus I/O
- UF iDataPlex ("*foxtrot*"). System operational for production Nimbus users. 10Gbps network enabled on the front-end and perfSONAR nodes.
- TACC Dell ("*alamo*").
    - OpenStack. New disk images created for server and nodes. Configured additional switch for public network. Installed Ubuntu on nodes for easier OpenStack installation.
    - XSEDE/slash2 Project. Demo'ed a slash2 file system test bed at SC12 (currently configured on 2 nodes from the HPC partition)
    - XSEDE software. Currently installing EMS test for GridFTP and Unicore. This will be the 3rd installation on Alamo for XSEDE Operations.

13.3.2 Services Activities (specific services are underlined in each activity below)

Accounting

XSEDE AMIE Gold integration

This will be a major development activity beginning in 2013, working in close collaboration with the AMIE Gold team.

FG Metrics

- Generation of a prototype statistic report generation framework with reports generated in PDF format. The report metrics, although very different from XSEDE, resemble them by providing simple summaries for multiple cloud services, clusters and FG projects. The switch of our charting tools to highcharts as Google charts were buggy and provided too little flexibility in terms of time series display.
- The design of a prototype real time FutureGrid resource monitoring table, which is similar to the XSEDE's resource monitor but for cloud services. It includes data from Nimbus, Eucalyptus, OpenStack, and HPC and shows utilization, running VMs, used and available cores, active users, projects and status are included to display
- Redesign of our real time FutureGrid resource monitoring for active FG users. It includes now the list of active users displayed in a different format on the web using Ajax/JSON

- Design of an analytics framework for project utilization. We designed a new module to provide resource usage information in terms of a project, a project leader and an institution
- Integration of the FG Metrics framework with OpenStack and Nimbus. Previously our framework was only displaying information for Eucalyptus.

Cloud Services and Support Software

Eucalyptus. With the release of Eucalyptus v3.1 the LDAP integration changed. This resulted in a significant update of the FG Eucalyptus/LDAP integration. There are now eucagroups and eucaaccounts OU entries in LDAP for each project.

Nimbus.

- Deployed Nimbus version 2.10 on *sierra*
- Developed and deployed new versions of Phantom, including:
  - sensor management, allowing to dynamically scale up and down collections of virtual machines from sensor metrics
  - multi-cloud support, allowing to deploy collections of virtual machines spanning multiple clouds
  - a new user interface
- Ongoing work with several groups to leverage Phantom and demonstrate it with various FutureGrid project use cases: Swift (FG-47), ATLAS (FG-298), University of Colorado Boulder (FG-121)
- Developed and released a new version of cloudinit.d, version 1.2, offering more customization options to the user:
  - providing support for custom SSH options
  - customization and management features for the working directory on deployed VMs
  - allows users to customize timeouts
  - allows users to run local commands from cloudinit.d launch plans
- Established daily collection of Nimbus metrics for the FG Cloud Metrics framework

OpenStack. In an evaluation we found out that the new version of OpenStack ("Folsom") has a new network component called Quantum that was not stable. However, we have set up Folsom's Nova Client, which gives more functionality to the users. In particular, the ability to make a snapshot from a running instance is very useful. We also started the testing of an LDAP integration with Folsom. The implementation of Keystone in Folsom works better than that in Essex. We are performing additional testing to determine whether we should put this into production. Furthermore, we are now also evaluating the next release of Openstack called "Grizzly" that introduces a new LDAP management package into OpenStack. The Grizzly release is anticipated to be available in April 2013. OpenStack has changed their 3 month release cycle to a 6 month release cycle due to the many changes that took place and prevent a potential production deployment.

Continued to investigate installing OpenStack on *alamo* during the quarter. A new version of OpenStack (Folsom) was released at the end of September and we switched our efforts to that version. We investigated a number of different hardware and software configurations and the result is an installation-in-progress of Folsom that uses the OpenStack Quantum networking software atop OpenVSwitch and KVM. A newly-acquired server is being used as the controller node with existing Alamo blade servers as compute nodes. All of these servers are running Ubuntu Linux since the CentOS Linux distribution is slower to include new versions of software such as OpenStack and OpenVSwitch. We are still debugging the networking part of this installation, so it is not yet available to users. Created a new tool and documentation that allows users to change their own password for the OpenStack dashboard.

ViNe. Improvements to ViNe software focusing on end-to-end overlay network performance. Specifically:

- The ViNe router module responsible to parse and execute commands issued by the ViNe management server has been revised to support long running commands.
- The internal data structure that maps external commands to internal APIs has been revised for improved performance. Instead of using hash-based data structure, an array of objects is currently used for faster access.
- ViNe routing table cache has been designed and implemented achieving improved (reduced) overlay messages/packets processing time. By avoiding the time consumed for hash processing, the designed routing table cache can deliver overlay routing information of a given ViNe node up to 100 times faster. This improvement translates to better ViNe router packet processing capacity (i.e., better end-to-end throughput and scalability).
- A ViNe module that manages Generic Routing Encapsulation (GRE) tunnels has been implemented and tested. Management APIs are now available to establish and tear-down GRE tunnels between ViNe routers. ViNe routers are required to have a public IP address in order to establish GRE tunnels, so not all ViNe routers can benefit from this feature. Connectivity and performance tests between *foxtrot* and *sierra* indicate that the kernel-based tunneling of GRE offers a better performance compared to user-level tunneling code.

Experiment Management

Experiment Harness. The Message-Based Execution and Management System (MEMS) requires a messaging infrastructure and benefits from resource information being available via messaging. The focus during this quarter has been to provide this infrastructure (see the Information Services section below).

Pegasus. To support higher level experiments, such as running workflow and other workloads, testing different filesystem setups and time-based repeatable experiments, a Python API was implemented. The name of the API is Pegasus Repeatable Experiments for the Cloud in Python, or Precip. The API provides flexible experiment management for running experiments on infrastructure clouds. Precip was developed for use on FutureGrid cloud platforms such as Eucalyptus (>=3.2), Nimbus, OpenStack, and commercial clouds such as Amazon EC2. The API enables users to easily provision virtual machines and run scripts and transfer data to/from sets of VMs identified by tags. The goal of the API is to provide a simple interface for writing repeatable experiments in Python.

The main feature of Precip is the ability to create repeatable, dynamic experiments programmatically. In Precip you can easily write code to start the deployment, add/remove VMs, run experiments, reconfigure, and shutdown cloud instances. The ability to express an experiment in code is also useful for experiments which have a time axis, or need to reconfigure the setup in response to events. A common use case is to remove or restart an instance at a particular time. Another is to grow the number of clients or servers over time. Precip tracks instances based on user and system supplied tags. The tags allow for group manipulation such as transferring files or running commands on a subset of VMs. The API does not require any special VM images or tools to be installed on those images. It can use any basic Linux image that supports SSH. Pre-configured images can be used if the experiment requires it, or the experiment API can be used to run bootstrap scripts on the images to install/configure required software. Precip has been installed on the India and Sierra FutureGrid resources. Documentation was added to the FutureGrid manual.

Image Management.

FG RAIN

We conducted a QA testing and refactored significantly the code improving software maintainability. We were able to reduce significantly the number of lines of code (25%). We conducted a redeployment of the new code.

FG teefaa

FG Teefaa is designed as a tool for System Administration to automate the system installation and operating system cloning. We experimented with the integrating of Torque/Moab scheduler to schedule OS provisioning with the help of teefaa. Significant changes in the design and in the code were made to enable the integration into Torque. This allows us to eliminate our previous dependencies on Moab. Testing is still ongoing. Teefaa is scheduled to be released next quarter.

Information Services

The FutureGrid messaging system provides a single location where users and tools can obtain a variety of information about FutureGrid. The various monitoring tools running on FutureGrid can publish information to the messaging system and users and tools subscribe to the messaging system for information of interest. Inca testing results and GLUE2 resource status information are currently being published to the messaging system and we plan to publish Ganglia system monitoring and perfSONAR network information.

During this quarter, we made fault tolerance improvements to the Inca plugins, made enhancements to the glue2 software, experimented with the CouchDB document-oriented database to store information received by the messaging system, and we started development on a Java helper API to make it easy to authenticate and subscribe to messages within Java applications.

HPC Services

Globus

The Globus GRAM 5 and GridFTP services continue to be available on *alamo* and *hotel*. At this time, these services are available to FutureGrid users upon request (we do not yet have an automated way for users to upload credentials to FutureGrid).

Performance

Inca. Improvements were made to the Inca plugin to publish Inca monitoring data to the FutureGrid messaging system. The enhancement allows for multiple RabbitMQ servers to be specified and will failover to an alternate server if the first is unavailable.

A new Inca test was written to test the EMI VM installed on the Xen Nimbus deployments on FutureGrid. The Inca test starts up an instance using the emi1-unicore-centos-5.3-x64-p1.gz VM image, submits a job to its EMI server and waits for the results, and then shuts down the VM instance.

The Inca team has been analyzing the Inca data collected on FutureGrid over the past few years, looking at test results from SSH, Cloud, and HPC tests to help motivate the design of better analysis tools for Inca.

PAPI. The PAPI team tested the upcoming release of PAPI 5.0 (aka PAPI-V) on Xen (Ubuntu 12.04) and KVM (CentOS 6.3) kernels, as well as an independent version of VMware 5.1 in preparation for release on FutureGrid. They also worked to develop a PAPI component for Infiniband in the virtual space as well as implementing improvements to the Appio component, used to measure I/O statistics in an application context

perfSONAR. The installation of all 10G cards ordered during the last quarter for the perfSONAR machines were completed and incorporated into the perfSONAR deployment to get a full mesh of 10G measurements. From this, two network performance problems (less than 1 Gbps) were noted from Chicago to India and from Chicago to Sierra. Both IU and SDSC are working to debug the cause of the problems at each of their sites.

FutureGrid Portal

- Established a Video/Multimedia Gallery in the FG Portal and launched this feature with a gallery dedicated to Science Cloud Summer School 2012 videos.
- Established and implemented new policies related to email notifications for FG Portal activities.
- Implemented a module to pull IU KnowledgeBase entries and create entries on FG Portal.
- Significant QA testing was performed as part of a refactoring of the outage email notice; project joining and leaving email notices.
- Significant update to the projects discipline classification. This included the design, implementation, and deployment of a new framework that eliminates errors that we saw due to issues in Google charts and the introduction of new categories

13.4 Security

No security issues occurred during this period.

13.5 Education, Outreach, and Training Activities

- FutureGrid at SC'12 in Salt Lake City:

  Monday November 12

  Tutorial: Infrastructure Clouds and Elastic Services for Science

  John Bresnahan, Argonne National Laboratory
  Kate Keahey, Argonne National Laboratory
  Patrick Armstrong, University of Chicago

Pierre Riteau, University of Chicago

Infrastructure-as-a-service cloud computing has recently emerged as a promising outsourcing paradigm: it has been widely embraced commercially and is also beginning to make inroads in scientific communities. Although popular, understanding how science can leverage it is still in its infancy. Specific and accurate information is needed for scientific communities to understand whether this new paradigm is worthwhile and how to use it. Our objective is to introduce infrastructure cloud computing and elastic tools to scientific communities. We will provide up-to-date information about features and services that benefit science and explain patterns of use that can best fit scientific applications. We will highlight opportunities, conquer myths, and equip the attendees with a better understanding of the relevance of cloud computing to their scientific domain. Our tutorial mixes the discussion of various aspects of cloud computing for science, such as performance, elasticity, privacy, with practical exercises using clouds and state-of-the-art tools..

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Tuesday November 13

BOF: Interoperability in Scientific Cloud Federations

Christine Morin, INRIA
Kate Keahey, Argonne National Laboratory
Yvon Jegou, INRIA
Roberto Cascellla, INRIA

The uptake of cloud computing has as major obstacle in the heterogeneity of hardware and software, which make difficult the portability of applications and services. Interoperability among cloud providers is the only way to avoid vendor lock-in and open the way toward a more competitive market. Interoperability can be achieved either by using open standards and protocols or by a middleware service to adapt the application/service to a specific cloud provider. The audience will be guided through the major challenges for interoperability from the IaaS to PaaS model and discuss the potential approaches for the interoperability in scientific cloud federations.

BOF: Computing Research Testbeds as a Service: Supporting large scale Experiments and Testing

Geoffrey Fox, Indiana University
José A.B. Fortes, University of Florida

This BOF discusses the concept of a Computing Testbed as a Service supporting application, computer science, education and technology evaluation usages that have different requirements from production jobs. We look at lessons from projects like Grid5000, FutureGrid, OpenCirrus, PlanetLab and GENI. We discuss 1) the requirements that Computing Testbeds as a Service need to address 2) The software needed to support TestbedaaS and a possible open source activity and 3) interest in federating resources to produce large scale testbeds and what commitments participants may need to make in such a federation.

Wednesday November 14

FutureGrid II Open Forum (morning session)

BOF: Science-as-a-Service: Exploring Clouds for Computational and Data-Enabled Science and Engineering

Manish Parashar, Rutgers University
Geoffrey Fox, Indiana University
Kate Keahey, Argonne National Laboratory
David Lifka, Cornell University

Clouds are rapidly joining high-performance computing system, clusters and Grids as viable platforms for scientific exploration and discovery. As a result, understanding application formulations and usage modes that are meaningful in such a hybrid infrastructure, and how application workflows can effectively utilize it, is critical. This BOF will explore how Clouds can be effectively used to support real-world science and engineering applications, and will discusses key research challenges (from both, a computer science as well as an applications perspective) as well as a community research agenda..

FutureGrid Booth Demos/Presentations/Q&A

FutureGrid II Open Forum (afternoon session)

- XSEDE Integration

  Enhance made to XSEDE site (www.xsede.org) to integrate information on FutureGrid:

  - Added new "Testbeds" option under Resources section, displaying summary information about FutureGrid
  - Added new "Testbeds" section to Resources Overview, displaying summary resource information about FutureGrid
  - In the Education & Outreach section, provided the appropriate description of and links to all videos from the VSCSE Cloud Summer School
  - Began implementing links to FutureGrid training materials from the XSEDE site

- Events this quarter (in order of most recent):

Type	Title	Location	Date(s)	Hours	Number of Participants	Number of Under-represented people	Method
Indiana University							
Presentation	Big Data and Clouds: Computing, Analytics and Curriculum	Persistent Systems Headquarters Pune India	12/20/2012	1.0	25		Live
Presentation	Introduction to FutureGrid: Towards a Computing Testbed as a Service	Instrumentation-as-a-Service for Computer and Information Science and Engineering	12/05/2012 to 12/06/2012	0.5	20		Live

		(INCISE 2) Workshop, Miami, FL					
Presentation	Reproducibility and Scalability in Experimentation through Cloud Computing Technologies	SC12, Salt Lake City, UT	11/14/2012	0.5	40		Live
Birds of a Feather	Computing Research Testbeds as a Service: Supporting large scale Experiments and Testing	SC12, Salt Lake City, UT	11/13/2012	0.5	40		Live
Birds of a Feather	Citrix CloudStack for Testbeds	SC12, Salt Lake City, UT	11/13/2012	0.5	40		Live
Birds of a Feather	Status of CNGrid and Interests on International Testbed	SC12, Salt Lake City, UT	11/13/2012	0.5	40		Live
Keynote	Large Scale Data Analytics on Clouds	CloudDB '12 Fourth International Workshop on Cloud Data Management, Maui, HI	10/29/2012	0.75	50		Live
Presentation	ACES and Clouds	APEC Cooperation for Earthquake Simulation (ACES) 8th International Workshop Advances in Simulation of Multihazards, Maui, HI	10/24/2012	0.25	30		Live
Keynote	Big Data in Research and Education	Symposium on Big Data Science and Engineering Metropolitan State University, Minneapolis, MN	10/19/2012	1.0			Live
Presentation	Cyber-Infrastructure Supporting Social Science	Internet2-Microsoft Workshop on Cyber-Infrastructure for the Social	10/16/2012	0.25	50		Live

		Sciences, University of Washington, Seattle, WA					
Presentation	Data Analytics and its Curricula	Microsoft eScience Workshop, 8th IEEE International Conference on eScience (eScience 2012), Chicago, IL	10/09/2012	0.50	30		Live
Presentation	Data Analytics and its Curricula	Delsa eScience Workshop, 8th IEEE International Conference on eScience (eScience 2012), Chicago, IL	10/09/2012	0.50	20		Live
Workshop	Cloud Computing for K-12	Introduction to High Performance and Cloud Computing for K-12 Teachers and Students, West Lafayette, IN	10/05/2012	2.0	18	6	Live
University of Chicago							
Birds of a Feather	Science-as-a-Service: Exploring Clouds for Computational and Data-Enabled Science and Engineering	SC12, Salt Lake City, UT	11/14/2012	1.0			Live
Birds of a Feather	Interoperability in Scientific Cloud Federations	SC12, Salt Lake City, UT	11/13/2012	1.0			Live
Tutorial	Infrastructure Clouds and Elastic Services for Science	SC12, Salt Lake City, UT	11/12/2012	8.0			Live
Presentation	Computing Power on Tap: Building an Outsourcing Ecosystem for Science	CLASS Conference, Bled, Slovenia	10/24/2012	1.0	~50		Live

University of Florida							
Keynote	Self-organizing Virtual Private Networks and Applications	Grid'5000 School, Nantes, FR	12/03/2012	1.0	~50		Live
Presentation	Peer-to-peer Virtual Private Networks and Applications	Vrije Universiteit Amsterdam, NL	11/08/2012	0.5	~20		Live

13.6 SP Collaborations

We have engaged in a collaboration with a cloud project in Europe (ConPaaS) which is considering the use of virtual machines based on the Grid appliance to support a task farming service.

13.7 SP-Specific Activities

See 1.3.2 Services Activities.

13.8 Publications

Shrideep Pallickara and Geoffrey Fox Recent Work in Utility and Cloud Computing Editorial of Future Generation Computer Systems Special Issue December 28 2012

Geoffrey Fox Large scale data analytics on clouds keynote in CloudDB '12 Proceedings of the fourth international workshop on Cloud data management Pages 21-24 October 29 2012 Sheraton Maui DOI

Jonathan Klinginsmith Reproducibility and Scalability in Experimentation through Cloud Computing Technologies Doctoral Showcase November 14 2012 SC12 International Conference for High Performance Computing, Networking, Storage and Analytics, Salt Lake City Utah November 10-16 2012

Saliya Ekanayake Survey on High Productivity Computing Systems (HPCS) Languages Technical report 13 November 2012

Manish Parashar, Geoffrey Fox, Kate Keahey Integrating Clouds and Cyberinfrastructure for CDS&E: Research Challenges Technical report October 26 2012

Hui Li, Geoffrey Fox, Judy Qiu Performance Model for Parallel Matrix Multiplication with Dryad: Dataflow Graph Runtime 2012 International Symposium on Big Data and MapReduce (BigDataMR2012) 01-03 November 2012, Xiangtan, Hunan, China

Geoffrey Fox, José A.B. Fortes Computing Research Testbeds as a Service: Supporting large scale Experiments and Testing Technical Report July 31 2012 Birds of a Feather on November 13 2012

at SC12 International Conference for High Performance Computing, Networking, Storage and Analytics, Salt Lake City Utah November 10-16 2012

Manish Parashar, Geoffrey Fox, Kate Keahey Science-as-a-Service: Exploring Clouds for Computational and Data-Enabled Science and Engineering Technical Report July 31 2012 Birds of a Feather on November 13 2012 at SC12 International Conference for High Performance Computing, Networking, Storage and Analytics, Salt Lake City Utah November 10-16 2012

Sherif Elmeligy Abdelhamid, Richard Alo, S. M. Arifuzzaman, Pete Beckman, Md Hasanuzzaman Bhuiyan, Keith Bisset, Edward A. Fox, Geoffrey C. Fox, Kevin Hall, S.M.Shamimul Hasan, Anurodh Joshi, Maleq Khan, Chris J. Kuhlman, Spencer Lee, Jonathan P. Leidig, Hemanth Makkapati, Madhav V. Marathe, Henning S. Mortveit, Judy Qiu, S.S. Ravi, Zalia Shams, Ongard Sirisaengtaksin, Rajesh Subbiah, Samarth Swarup, Nick Trebon, Anil Vullikanti, and Zhao Zhao CINET: A CyberInfrastructure for Network Science Technical Report July 19 2012 and Proceedings of 8th IEEE International Conference on eScience (eScience 2012) Hyatt Regency Chicago, Chicago, Illinois, 8-12 October 2012

13.9 Metrics

13.9.1 Standard systems metrics

Top 35 HPC FutureGrid Users #Jobs run (Oct-Dec 2012) - largest to smallest

Area	User	# Jobs	Avg Job Size (cpus)	Avg Wait Time (h)	Wall Time (d)	Avg Mem (MB)
University of Virginia	kasson	2480618	1	0	860.2	1.4
University of Virginia - Genesis	xcguser	589690	1	0.8	24169.4	99.1
University of Buffalo	charngda	185986	16.3	3.3	15889	68.4
University of Virginia - UNICORE	unicore	34010	1.6	0.1	595.8	8.3
Pittsburgh Supercomputing Center	vizino	29947	1	0	4.4	2.9
SDSC - INCA	inca	28081	6	2.4	1488.2	10
Oak Ridge National Laboratory	jychoi	10098	1.7	2	883	181.5
Technische Universität Dresden	williath	5598	1	6.2	594.2	22.8
University of Virginia	pela3247	5297	32.9	17.4	107328.8	501.7
LSU - SAGA	pmantha	3208	24.2	0.1	2300.4	134.3
LSU - SAGA	oweidner	2872	7.8	0.2	155.1	334.8
University of Massachusestts	dshrestha	1795	43.3	4.5	5436	659.6
Emory University	sagravat	1604	1.7	0	13.7	156.6
University of Notre Dame	dthain	1290	1	0	24.4	5.8
University of Utah	jasonkwan	1240	7	2.5	3184.3	47671.5
Univeristy of Southern California	weiyin	799	36.2	0.8	852.1	335.6
Indiana University	ktanaka	693	8.8	0	20.6	13.6
LSU - SAGA	ssarip1	656	42.5	0.4	1487.4	38.1
University of Piemonte Orientale	sguazt	565	1	0.1	415.7	1497.8
Indiana University	gaoxm	507	59	1	2693.8	178
Ruthers University	jdiaz	495	15.9	0	4.9	14.7
Indiana University	sbpatil	470	14	0	48.3	26.3
University of Notre Dame	pdonnelly	461	1	0	1.8	6.6
Indiana University	qismail	433	13.7	0	76.7	70.5
University of Florida	zincum	392	25.3	0.9	33.9	12017.4
Indiana University	nvkulkar	386	4	0	2.4	37.7
Ruthers University	azebro1	384	49.1	0.6	105.7	3254.7
Indiana University	bhasjais	373	14.9	0	72.3	32.3
Indiana University	ppudakal	372	11.8	0	36.3	57.1
University of Notre Dame	dpandiar	349	1	0	18.1	11.7
Juelich Supercomputing Centre	msmemon	343	2.5	0	0.3	2.3

13.9.2 Standard systems metrics (continued)

Top 30 HPC (Average) Memory Users - Largest to Smallest

Area	User	# Jobs	Avg Job Size (cpus)	Avg Wait Time (h)	Wall Time (d)	Avg Mem (MB)
University of Utah	mzachariah	5	8.2	2.3	4.5	107505.5
University of Utah	jasonkwan	1240	7	2.5	3184.3	47671.5
University of Utah	diarey	13	8	0	23	41150.8
Indiana University	ajyounge	44	8.7	0.6	1234	19231.3
Indiana University	upitamba	81	11.6	0	84.7	16050.3
University of Florida	zincum	392	25.3	0.9	33.9	12017.4
University of Southern California	cwickram	171	27.7	0.2	75.5	11891.2
Indiana University	nnmahaja	60	11.5	0	28.2	8413.7
University of California - Davis	emheien	7	43.4	0	42.5	4803.8
University of Chicago	leggett	177	66.1	0.1	34.2	4616.9
Ruthers University	azebro1	384	49.1	0.6	105.7	3254.7
Indiana University	crajacks	44	2.4	1.2	11.8	2336.5
University of Piemonte Orientale	sguazt	565	1	0.1	415.7	1497.8
Indiana University	xc7	5	8	0.8	7.1	859.3
TACC	wsmith	208	17.6	0	2552	839.6
LSU	nykim	139	21.1	1.3	169.7	695.7
University of Massachusestts	dshrestha	1795	43.3	4.5	5436	659.6
Indiana University	adnanozsoy	139	1.8	2.1	10.1	635
Rutgers University	gdiaz	62	14.1	28.7	5.8	537.5
University of Virginia	pela3247	5297	32.9	17.4	107328.8	501.7
University of Florida	bpareek	1	32	4.6	10.7	474.1
Indiana University	shrray	109	9	0	439.7	454.4
University of Central Florida	anthony	26	15.6	0.2	6.8	444.2
Indiana University	xqiu	8	4.3	0	3.8	432.8
Indiana University	lihui	331	19.8	4.1	1616	428
Indiana University	jiang28	124	15.8	0.7	33.4	400.1
University of Central Florida	szittrower	16	32	0	33.6	383.4
Emory University	ablimit	198	158.3	1.2	3267.7	371.6
University of Florida	nehauppal4	3	32	3	10.8	370.6

13.9.3 Standard systems metrics (continued)

Top 30 HPC (Average) Job Size Users - Largest to Smallest

Area	User	# Jobs	Avg Job Size (cpus)	Avg Wait Time (h)	Wall Time (d)	Avg Mem (MB)
Indiana University	dtuncay	1	232	3.3	11.8	229.1
Indiana University	feiteng	2	232	0.1	313.7	36.2
Emory University	ablimit	198	158.3	1.2	3267.7	371.6
indiana University	azadeh	10	156	41.5	3488	19.4
Indiana University	yuduo	15	137.1	0	876.3	31.3
Indiana University	zhguo	37	130.1	17.5	18323.7	2.7
Indiana University	weng	89	123.5	6.5	7641.6	21.4
indiana University	yangchen	36	79.1	0.1	2414.5	24.8
University of Chicago	leggett	177	66.1	0.1	34.2	4616.9
Indiana University	gaoxm	507	59	1	2693.8	178
indiana University	sekanaya	7	52.7	0	191.3	249.7
Ruthers University	azebro1	384	49.1	0.6	105.7	3254.7
University of Florida	shekar9	29	47.7	0	2.9	116.2
University of Florida	bhargavuln	45	43.6	0	57.1	140.3
University of California - Davis	emheien	7	43.4	0	42.5	4803.8
LSU - SAGA	luckow	272	43.4	0.3	302.9	178
University of Massachusestts	dshrestha	1795	43.3	4.5	5436	659.6
University of Florida	yagarwalla	6	42.7	1.1	11.5	297.9
LSU - SAGA	ssarip1	656	42.5	0.4	1487.4	38.1
Indiana University	yangruan	40	37.3	85.7	1076.2	207.1
University of Florida	revanth109	46	36.4	0	1.7	77.4
Univeristy of Southern California	weiyin	799	36.2	0.8	852.1	335.6
University of Florida	syam	4	36	0	0.2	90.7
University of Florida	deepakdas	29	34.2	3.3	2.5	221
University of Florida	kabhishe	51	33.9	5.5	1.2	100.8
University of Virginia	pela3247	5297	32.9	17.4	107328.8	501.7
University of Florida	aphukan	26	32.3	0	280.8	85.7
YunNan University, CHINA	anny	2	32	17.4	0	0.7
University of Florida	anurag.sharma	19	32	0	5.6	91.5

13.9.4 Standard User Assistance Metrics

RT Ticket System

New/Open tickets (210) in period, grouped by queue (category):

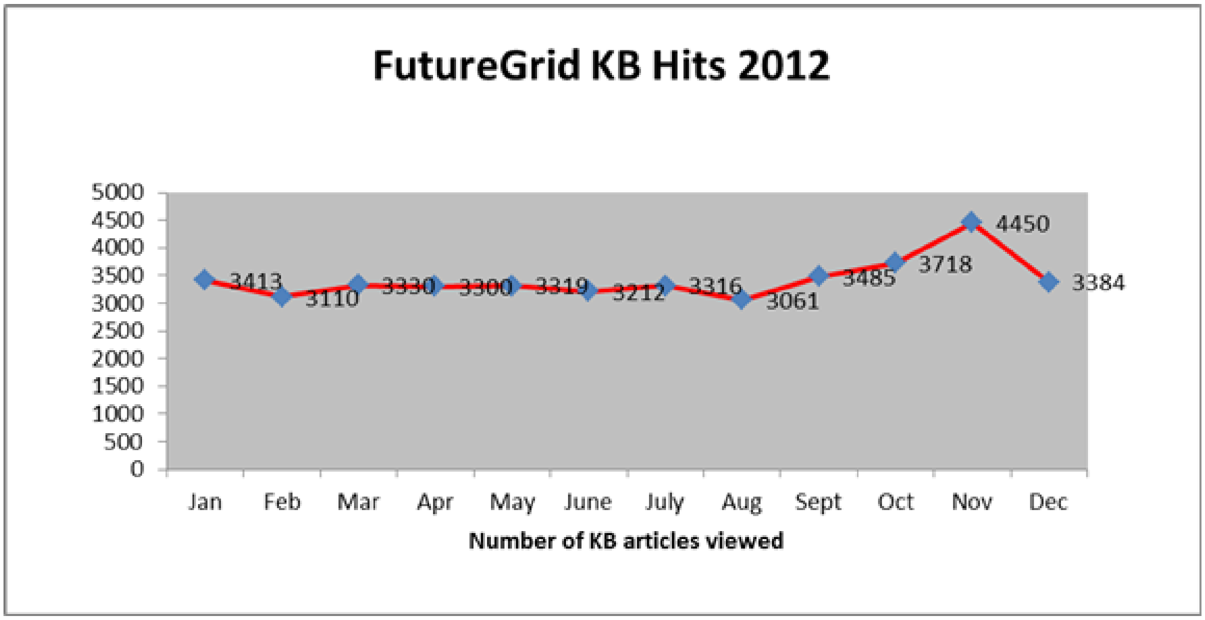
a) 006 FutureGrid account requests
b) 009 Portal account requests
c) 004 Eucalyptus issues
d) 020 Nimbus issues
e) 011 OpenStack issues
f) 124 General issues
g) 014 *hotel* issues
h) 008 *alamo* issues
i) 005 *xray* issues
j) 007 User Support issues
k) 002 Systems issues

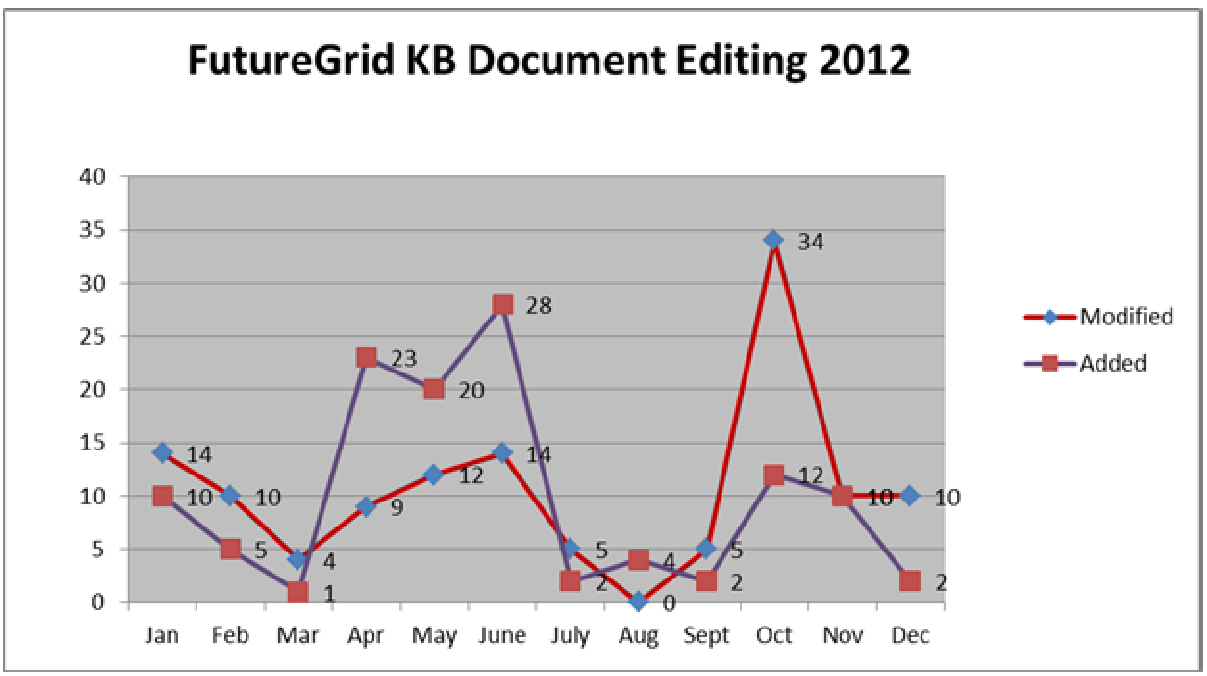
Resolved tickets (188) in period, grouped by queue (category):

a) 003 FutureGrid account requests
b) 006 Portal account requests
c) 006 Eucalyptus issues
d) 021 Nimbus issues
e) 010 OpenStack issues
f) 109 General issues
g) 015 *hotel* issues
h) 007 *alamo* issues
i) 005 *xray* issues
j) 006 User Support issues

13.9.5 <u>SP-specific Metrics</u>

Knowledge Base:





Projects:

- Twenty-three (23) new projects added this quarter (289 total projects)
- Categorization of projects to date:

  a) Project Status:
  Active Projects: **256(88.6%)**
  Completed Projects: **20(6.9%)**
  Pending Projects: **0(0%)**
  Cancelled Projects: **1(0.3%)**
  Incomplete Projects: **0(0%)**
  Denied Projects: **12(4.2%)**

  b) Project Orientation:
  Research Projects: 228(82.3%)
  Education Projects: 46(16.6%)
  Industry Projects: 2(0.7%)
  Government Projects: 1(0.4%)

  c) Project Primary Discipline :
  Computer Science: 144(49.8%)
  Technology Evaluation: 24(8.3%)
  Life Science: 29(10%)
  Education: 40(13.8%)
  Interoperability: 10(3.5%)
  Domain Science excluding Life Science: 27(9.3%)
  Not Assigned: 3(1%)

  d) Project Service Request/Wishlist:

  High Performance Computing Environment: **144(49.8%)**
  Eucalyptus: **147(50.9%)**
  Nimbus: **149(51.6%)**
  OpenStack: **79(27.3%)**
  OpenNebula: **56(19.4%)**
  Hadoop: **106(36.7%)**
  Twister: **42(14.5%)**
  MapReduce: **100(34.6%)**
  Genesis II: **31(10.7%)**
  XSEDE Software Stack: **51(17.6%)**
  Unicore 6: **18(6.2%)**
  gLite: **21(7.3%)**
  Vampir: **15(5.2%)**
  CUDA(GPU Software)): **11(3.8%)**
  SAGA: **3(1%)**
  Globus: **21(7.3%)**
  Pegasus: **17(5.9%)**
  PAPI: **16(5.5%)**
  MPI: **18(6.2%)**
  ScaleMP: **4(1.4%)**

14 Indiana University Pervasive Technology Institute - Service Provider Quarterly Report

14.1 Executive Summary

During the current quarter, IU continued hosting its Level 2 and Level 3 (Pending) systems – the Quarry virtual machine (VM) hosting and Rockhopper. Perhaps the most significant change in our service offerings during the current reporting period is that IU applied for and was granted "NET+ Evaluation" service status by Internet2. NET+ services represent a large scale effort by Internet2 to achieve the economy of scale of large vended (often cloud) solutions while retaining a significant amount of institutional control over license terms and quality of service. NET+ services are all well publicized within the Internet2 community and one set of terms is negotiated with Internet2, applicable to all users. NET+ services also come with an interesting usability requirement: authentication via InCommon credentials is a required characteristic of NET+ services. Becoming registered as a NET+ service identifies this service to an important constituency that – as a group – is likely to find it easier to discover a NET+ Service than an Internet2 service. (More information is available at www.internet2.edu/netplus/.)

Normal operational activities proceeded routinely and without incident.

There were many significant educational and outreach activities carried out during this reporting period. Among the most significant outreach activities were an RNA sequence assembly workshop at the World Genome Data Analysis conference in San Francisco and presentations at the annual meeting of the American Geophysical Union. These are important efforts to reach out to mainstream domain scientists at the domain science conferences rather than speaking to the few domain scientists that come to computational science conferences. An important part of our work this quarter was preparation for an exhibit/booth at the Plant and Animal genome conference which takes place in January 2013.

Efforts at computational science conferences were highly successful – particularly the IU display at SC12. This display was a significant success, including a novel and interesting demonstration of new data transport technology. Indiana University collaborated with Technische Universitaet Dresden and Orange Telecommunications to demonstrate RDMA (Remote Direct Memory Access) over Converged Ethernet (RoCE) across a wide area network using the Lustre file system at the SC12 display. This was led technically by D. Martin Swany, Stephen Simms, and Matt Davy. This memory-to-memory copying of data presents tremendous possibilities for distributed parallel computing.

14.1.1 Indiana University Level 2 Service Provider Systems: Resource Descriptions

Level 2 - Quarry Virtual Machines - The Quarry Gateway Web Services Hosting resource at Indiana University consists of multiple Intel-based HP systems geographically distributed for failover in Indianapolis and Bloomington, IN. Currently there are four HP DL160 front-end systems at each site. Each is configured with dual quad-core Intel E5603 processors, 24 GB of RAM, and a 10-gigabit Ethernet adapter. There are a total of 48 XSEDE VMs. The front-end systems host the KVM-based virtual machines. VM block storage is provided by two HP DL180 servers at each site configured with a quad-core Intel X5606 processor, 12 GB of RAM, a 10-gigabit Ethernet adapter, and a RAID controller attached to an HP storage array. Quarry is used solely for hosting science gateway and web service allocations, or services to support central XSEDE infrastructure. Requests are restricted to members of approved projects that have a web service component.

Level 3 (Pending) - Rockhopper - Rockhopper is a collaborative effort between Penguin Computing, IU, the University of Virginia, the University of California Berkeley, and the University of Michigan to provide supercomputing "cluster on demand" services in a secure US facility. Researchers at US institutions of higher education and federally funded research centers can purchase computing time from Penguin Computing and receive access via high-speed national research networks operated by IU. It takes just minutes to go from submitting credit card information via a web form to computing on Rockhopper (the system itself is owned by Penguin; cycles on Rockhopper are purchased from Penguin). Rockhopper is a 4.4 TFLOPS system based on AMD processors.

14.2 Science Highlights

14.2.1 RDMA (Remote Direct Memory Access) over Converged Ethernet (RoCE) across a wide area network using the Lustre file system Demonstration at SC12.

Science is driven by big data and its potential. From understanding the laws of nature to creating drugs to combat disease, the ability to quickly move and share data with colleagues around the world is critical to scientific success. In a recent breakthrough, Indiana University networking experts, in collaboration with Orange Telecommunications and DataDirect Networks, proved that data sharing can be faster, more efficient and more cost effective.

Figure 1. Collaboration team displaying successful demonstration of 40 gigabytes per second of RDMA over Converged Ethernet (RoCE) in Indiana University booth at SC12.

At the annual International Conference for High performance Computing, Networking, Storage and Analysis, the collaboration team performed the world's first 40 gigabytes per second demonstrations of RDMA over Converged Ethernet (RoCE) in a wide area network using the Lustre file system. RoCE, pronounced "Rocky," is a network protocol that enables remote direct memory access over an Ethernet network. In addition to accelerating data transfer, RoCE has the potential to further the possibilities of software-defined networking (SDN). RoCE requires guaranteed bandwidth and SDN makes it possible to dynamically allocate bandwidth in the WAN in response to the needs of the application.

14.2.2 Education, Outreach, and Training highlight – IU display at SC12

Indiana University's booth titled "Mapping Innovation, Bridging to the Future" at the annual Supercomputing Conference offered talks, demonstrations, and live interactive hardware for visiting researchers, agency officials and potential collaborators. This year featured demonstrations of 3-D printing, facial recognition, pipe organs, and the ever-popular World View networking display, along with the featured IQ Tilt-table.

Figure 2. Visitors to the IU booth interact with a wide range of visualization projects on the IQ Tilt-table.

This year's booth showcased IU research partnerships with America Connects to Europe (ACE) and GEANT, the pan-European data network. Orange Telecommunications and DataDirect Networks, Inc. also partnered with IU staff in a "world's first" demonstration of Remote Direct Memory Access over Converged Ethernet (RoCE) across a wide area network using the Lustre file system. This demo showed that data sharing can be faster and more efficient over wide area networks.

14.3 User-facing Activities

14.3.1 System activities

14.3.1.1 Level 2 – Quarry (virtual machines)

During Q4 a new 36TB storage array was added to the Quarry Gateway Hosting service hardware located at IUB and the storage controller was upgraded to match the hardware at IUPUI.

14.3.1.2 Level 3 (pending) – Rockhopper (Penguin on Demand commercial cluster as a service)

There were no issues with Rockhopper during this quarter.

14.3.2 Services activities

14.3.2.1 Level 2 – Quarry

No changes were made to the Quarry VM service this quarter.

Quarry continues to be used solely for hosting science gateway and web service allocations, or services to support central XSEDE infrastructure. Requests are restricted to members of approved projects that have a web service component. An external request form can be found at: *http://pti.iu.edu/hps/vm-account-request*.

14.3.2.2 Level 3 (pending) – Rockhopper

The Rockhopper service saw an increase in usage during the Q2 of PY2. There were 2,022 user logins recorded, and 44,543 jobs were run. In addition, 9 new users were added to the system, increasing the total to 80.

14.4 Security

There were no security issues during the reporting period.

14.5 Education, Outreach, and Training Activities

Type	Title	Location	Date(s)	Hours	Number of Participants	Number of *Under-represented people	Method
Conference talk/presentation/panel	Celebrate Science Indiana	Indianapolis, IN	6 Oct-12	8 hours	2500	500	S
Workshop	RFS Training Workshop - Nursing	IU Indianapolis, IN Campus	15 Oct-12	2 hours	23	2	S
Workshop	Galaxy Workshop	IU Bloomington, IN Campus	19 Oct-12	6 hours	111	5	S
Conference talk/presentation/panel	SC12 Conference	Salt Lake City, UT	12-15 Nov-12	24 hours	4000	1000	S
Workshop	GIS Day at Indiana University	Bloomington, IN	14 Nov-12	5.5 hours	400	100	S
Workshop	RNA Sequencing Workshop	World Genome Data Analysis, San Francisco, CA	26 Nov-12	3 hours	8	1	S
Conference talk/presentation/panel	The Apache Software Foundation, Cyberinfrastructure and Scientific Software: Beyond Open Source RNA-Sequencing	Salt Lake City, UT	13 Nov-12	1.5 hours	50	10	S
Conference talk/presentation/panel	Realizing the universe on XSEDE	ECSS Symposium, Bloomington, IN	18 Dec-12	0.5	20	1	V
Conference talk/presentation/panel	Open community software: Building science gateways and workflows	SC12, Salt Lake City, UT	12-14 Nov-12	1.5	20	3	S
Conference talk/presentation/panel	Open community software: Building science gateways and workflows	JSMF Workshop, Bloomington, IN	16-17 Nov-12	0.5	10	1	S
Conference talk/presentation/panel	Building Scientific Workflows for the Geosciences with Open Community Software	American Geophysical Union, San Francisco, CA	7 Dec-12	0.5	25	5	S

Table 1. EOT activities for Q4 of Calendar 2012. *Traditionally underrepresented groups.

14.6 SP Collaborations

Indiana University collaborated with Orange Telecommunications and DataDirect Networks (in an international and public / private partnership) to demonstrate RDMA (Remote Direct Memory Access) over Converged Ethernet (RoCE) across a wide area network using the Lustre file system, described above under Science Highlights.

14.7 SP-Specific Activities

Data Services (WBS 1.2.2)

File system support

Justin Miller has worked with the other members of the XSEDE-wide Albedo file system administration team to bring the service to retirement. Justin continues to support XSEDE users who are using Data Capacitor resources primarily through gateway allocations.

Systems Operational Support (WBS 1.2.6)

Virtual machines

IU staff provided ongoing operational support for virtual machines (VMs) hosted on the IU Quarry system. IU staff are also completing the installation of a central XSEDE Nagios deployment.

During the current quarter, the IU Gateways team worked on issues regarding gateway operations and XSEDE middleware that cut across several gateway efforts. IU XSEDE staff worked with system administrators and grid middleware (GRAM 5) providers to continue effort on improving error propagation from XSEDE resources to end users through Gateway middleware. This included in particular the following activities:

- Better notification of application errors to the gateway by parsing Stderr Parsing. Gateway middleware typically rely on exit codes to determine the application execution success/failure. Often this is not foolproof as MPI job exit codes are misleading. IU staff enhanced crosscutting gateway middleware to parse the Standard Error and Standard Out to more reliably determine application success.
- Gateway Test Clients: IU XSEDE staff initiated an effort to develop standalone grid test clients. The lack of simple-to-use, reproducible test sandboxes makes it cumbersome and sometimes impossible to identify and resolve grid middleware failures. This quarter the effort focused on simple GridFTP and GRAM test clients, which led to a larger discussion on the need for and usefulness of such clients. For reference, the simple clients are publicly available to download and use:
    - https://svn.apache.org/repos/asf/airavata/sandbox/grid-tools/gram-client/
    - https://svn.apache.org/repos/asf/airavata/sandbox/grid-tools/gridftp-client/

XD Operations Center Fail-over

In the event of an emergency and/or an extended outage, Indiana University's GlobalNOC (Global Research Network Operations Center) will serve in the role of a backup XNOC. GlobalNOC is located in Indianapolis on the IUPUI campus. GlobalNOC will be prepared to receive/send emails that are directed to help@xsede.org. In addition, GlobalNOC set up a dedicated phone line at (317) 274-7782 and is prepared to take phone calls directed to XNOC should the primary XOC at NCSA be unreachable due to an emergency and/or an extended outage.

The list below includes items on which we have made significant progress, and which should be completed in Q1 of 2013:

- Phones: An XSEDE NOC greeting was added on the IU phone system, and we are waiting on the pending toll-free provider redirecting the number and process. Details are still being worked out as far as who should be authorized to request a pull of the phone to be answered by GlobalNOC. XNOC will initiate a push for all the incoming calls if need be during an emergency and/or an outage.
- Email: Setup of email acceptance for failover on the IU GlobalNOC side is awaiting XSEDE/NCSA setup, policy and procedures, and documentation before we continue. An inbox is already set up, but a process/procedure is still in the works to determine how email can be pushed to GlobalNOC and by whom.

The list below includes items that are on hold pending decisions by XSEDE management:

- Ticketing: GlobalNOC awaits announcement of a final decision on a new trouble ticket system for XNOC. A shared account has been created for GlobalNOC to have access to the ticketing system once a decision is made as far as what ticketing system to use. The current timeline for the new ticketing system implementation is Q2 of 2013.
- Monitoring: Still pending; we are waiting on a setup to access current XNOC monitoring.
- Process and Procedure Documentation: GlobalNOC is still waiting on centralizing all XSEDE documentation to the XSEDE Staff Wiki.
- Fail-over Documentation: If process/procedure documentation is centralized into the staff wiki, then the fail-over process for documentation will become part of the overall fail-over process.
- Training: GlobalNOC staff needs to receive training from XNOC on trouble ticket system usage and/or other tools that will be needed during an emergency and/or an extended outage.
- XNOC Staff relocation: This item is still in the works. If need be, XNOC staff can relocate to GlobalNOC to work at Indianapolis during an extended XNOC outage.

User Information and Interfaces (WBS 1.3.2)

Documentation

During Q4, work began on an initial Mason User Guide for the XSEDE site, working with Susan Lindsay on several iterations. Multiple docs were added to IU internal XSEDE wiki for preservation. In adding docs, it was necessary to create some additional categories and apply new organization to some archives. A section for EOT activities was added and populated and preliminary work on an email2wiki gateway begun to automate the process between RequestTracker, where EOT items are entered, and the wiki for archiving. An archive for IU XSEDE meeting minutes was created. Completed work with PSC and Maytal to store a large XSEDE12 organization archive and also stored it locally to IU wiki. Work began with NCGAS on their web presence to set up a portal page for Galaxy; an XSEDE science gateway resource. Editorial staff in the grant support area have been heavily involved in editing all campus bridging documents before distribution and/or publication to public facing outlets. This editing serves a very important function in the document creation process, by adding clarity and readability of documents intended for wide distribution to this new EOT area of XSEDE.

User Engagement (WBS 1.3.3)

Annual User Satisfaction Survey

Planning for the 2013 User Satisfaction Survey began in November 2012, and a preliminary draft for review and comment was provided to Level 2 and 3 managers in mid-December. All feedback has been reviewed and, with few exceptions, incorporated into a final draft that will be shared with the Senior Management Team (SMT) during the week of January 14. Simultaneous to SMT review, documents will be submitted to the IU Institutional Review Board for exempt study approval. The survey is on target to launch in late January 2013, with preliminary results available for review at the March 2013 quarterly meeting. Key changes to the 2013 survey are as follows:

The survey will be much shorter in length, allowing respondents to complete the survey in 10 minutes or less.

The annual user satisfaction survey will be confined to broad, crosscutting issues that are of interest to all users, with the aim of providing a "report card" to service owners about satisfaction with the fundamental dimensions of their service or resource.

To gauge satisfaction with specific resources and services used by smaller subsets (e.g., ECSS, Allocations, etc.), short, targeted "point-of-service" surveys, interviews, and focus groups will be conducted throughout the year, pending additional funding and IRB approval.

Efforts to weight the random sample of potential respondents so as to correlate with the overall XSEDE population are underway. (For example, if the overall XSEDE population is 20 percent post-doctoral fellows, the sample survey population should include roughly 20 percent post-doctoral fellows, and so on.) This is dependent upon whether this information is recorded and readily available from XSEDE.

Additional publicity efforts will be made to increase the response rate, with the goal of achieving a 30 percent response rate. These efforts include multiple reminders, notices on the XSEDE portal (proposed) and messaging in the monthly XSEDE newsletter.

Efforts will be made to standardize certain language and questions across multiple survey efforts in other areas (e.g., Community Requirements and TEOS) for consistency, and to allow for easier cross-referencing and the potential reuse of existing data.

Novel & Innovative Projects (WBS 1.4.2)

Pierce presented XSEDE Science Gateways and workflows at the JSMF Workshop on Plug-and-Play Macroscopes meeting (http://scimaps.org/meeting/121116/) held in Bloomington, IN November 16-17. The goal of this workshop was to examine cyberinfrastructure requirements for Library Sciences. Prof. Katy Borner from Indiana University School of Library and Information Science is potentially a significant user of XSEDE resources. IU ECSS NIP staff will follow up to see if she is interested.

Extended Support for Science Gateways (WBS 1.5.2)

Gateway Management

Summary: The IU team continued its role of leadership of the XSEDE Science Gateway program. Major efforts included the organization of interleaving biweekly meetings. The gateways staff calls occur on alternating weeks and focused this quarter on use cases and common middleware requirements, discussed in more detail below. The IU team also organizes open, biweekly symposia on gateways and gateway-related efforts. Presentation topics included cybersecurity from Von Welch, the MyHadoop work at SDSC, and the Computational Infrastructure for Geodynamics Seismology Portal by Eric Heien. Also during this period, the IU gateways team devoted significant effort to the science gateways and scientific workflow use case discussions with the XSEDE Architecture and Design team. Detailed tasks include:

- Working with the Architecture and Design team to finalize five gateway use cases. This exercise is resulting in an extensive survey of gateway architecture in regards to XSEDE integration. The effort was coordinated through contributed use cases from teleconferences.
- Working with the gateway community in developing a gateway cookbook with recipes of various gateway-building exercises. This quarter focused on laying out an outline agreeable to all gateway contributors. For reference, the outline and timeline are described at https://docs.google.com/document/d/1sv2XjHW-Q41KqKgEF-tSLSo1ZcdCLIwimSK3ELm_tbg/edit#heading=h.u87mnyd8s3dp
- Submitted new areas of gateway focus to XSEDE Management. Brief summary of two requests:
    - Develop gateways for popularly used community codes in order to meet the NSF mandate of broadening XSEDE impact through gateways.
    - Bootstrap a Cyberclient community for gateway developers to share codes and experiences in using XSEDE middleware.
- Continued discussions with XSEDE Architects in strategizing gateway transition to emerging XSEDE Architectural components.
- Worked with Trestles Grid Administrators in testing and validating GRAM5 job management service.

Gateway Operations & XSEDE Grid Middleware Reliability Improvement

During the current quarter, the IU Gateways team worked on issues regarding gateway operations and XSEDE middleware that cut across several gateway efforts.

- Working with system administrators and grid middleware (GRAM 5) providers to continue effort on improving error propagation from XSEDE resources to end users through Gateway middleware.
- Better notification of application errors to gateway by parsing Stderr Parsing:
    - Gateway middleware typically rely on exit codes to determine the application execution success/failure. Often this is not foolproof as MPI job exit codes are misleading.
    - Enhanced crosscutting gateway middleware to parse the Standard Error and Standard Out to determine application success.
- Gateway Test Clients: Initiated an effort developing standalone grid test clients. The lack of simple-to-use, reproducible test sandboxes makes it cumbersome and sometimes impossible to identify and resolve grid middleware failures. This quarter the effort focused on simple GridFTP and GRAM test clients but this effort led to a larger discussion on the need and usefulness of such clients. For reference, the simple clients are publicly available to download and use from:
    - https://svn.apache.org/repos/asf/airavata/sandbox/grid-tools/gram-client/
    - https://svn.apache.org/repos/asf/airavata/sandbox/grid-tools/gridftp-client/

IU ECSS Supported Projects

The IU XSEDE team supported the following ECSS projects:

- ***OLAM Final Report***
  - Summary: We concluded the OLAM ECSS project. Project PI Craig Mattocks refocused storm surge and climate simulation efforts because of stalled external development efforts of the OLAM model. Dr. Mattocks was able to use XSEDE resources in similar calculations using the Advanced Hurricane version of WRF model and used the Gordon cluster to generate a Storm Surge Simulation initialized with a SWARN near wave shore wave mode. Initial results on hurricane Sandy led to refocused activity of SLOSH-SWARN workflows from Dr. Mattock's team.
- ***Dark Energy Survey***
  - Summary: Our efforts during this reporting period were a) to move the workflow execution to Trestles from Ranger because of Ranger's retirement and b) to run production Dark Energy Survey (DES) workflows. The IU team worked with SDSC system administrators to enable DES jobs on Trestles. This involved testing the Grid middleware on Trestles and resolving differences between the Ranger and Trestles computational environments. Two significant issues needing resolution were module loading and configuration issues to run MPI jobs. PBS jobs have only /scratch folder write permission on Trestles, but for DES applications required creating a shared folder for sharing intermediate input/output files for a set of jobs in a workflow before running a job. To resolve this, SDSC system administrators created a special scratch location for DES projects, based on requirements provided by the IU team. The IU team also assisted DES researchers with the execution of two production workflows (identified as "Beluga" and "Chinchilla" within the group) on Ranger, which produced 30 TB of data and consumed 600,000 SUs. Data were moved to SLAC for post processing. Production workflow results are made available from SLAC to the DES scientific community and published as a catalog for the Blind Cosmology Challenge. This work was described in an ECSS-wide symposium presentation by IU's Raminder Singh.
  - Objectives: Migrate DES workflow to Trestles from Ranger. Run production DES runs.
  - Detailed tasks performed include:
    - Migrated code to Trestles to run simulation to extend the production scope.
    - Tested the code on Trestles and the option to utilize 1024 cores to run large simulations.
    - Ran into PBS scripts issue with MPI libraries having different syntax to configure such jobs.
    - File system issues were reported on Trestles' compute nodes while running the large simulations.
    - Ran two production runs on Ranger: Beluga and Chinchilla, which produced 30 TB of data and consumed 600,000 SUs. Data were moved to SLAC for post processing.
    - Updated the gateway middleware to the latest available general-purpose gateway middleware Airavata workflow. The middleware is now hosted on XSEDE gateway hosting VMs at IU.

        - XSEDE Globus GRAM submissions are initiated through a recommended JGlobus library. The jobs managed through this client have seen occasional failures for long running jobs; a precise reason could not be determined. Working with TACC Admins and Globus Developers, the temporary resolution was to disable the job cancellation features in the JGlobus Clients. This addressed the failures and moved forward the DES project. A permanent fix is needed. The problem and temporary resolution are recorded in the XSEDE ticket number # 220803.

- ***VLAB***
    - Summary: VLAB support activities were minimal during this quarter because of the unavailability of the primary VLAB developer. The IU team was able to reach the developer near the end of the reporting period and did make progress on some technical issues described below.
    - Objectives: To enable the VLAB gateway to submit jobs and workflows to XSEDE resources.
    - Detailed activities concluded during this reporting period include:
        - Continued work with primary VLAB developer on integrating their portal with current version of Apache Airavata gateway middleware. This will allow VLAB to outsource migration to different XSEDE resources to the IU gateways team.
        - Improved the gateway specifying a local file as an input staging URL. The gateway previously only supported GridFTP URLs for input file transfers. The effort involved testing local file protocols in the gateway job submission clients.
        - Investigating ways to support VLAB on Stampede.
- ***UltraScan***
    - Summary: IU ECSS assisted with the UltraScan team with the transition of its applications and gateway middleware from Ranger to Trestles. This involved significant operational testing of Trestles' middleware, which was documented in several XSEDE tickets. The IU ECSS team also assisted with the maintenance of the UltraScan team's campus bridging middleware.
    - Objectives: Support the transition of UltraScan applications and middleware to use Trestles.
    - Detailed activities concluded during this reporting period include:
        - Helped to update XSEDE InCommon certificates on one of local (campus) cluster.
        - Helped with following XSEDE failures:
            - Ticket # 221729: Connection failure to submit a job on Lonestar. There was a firewall issue that disappeared after some time. The consulting TACC administrator was not able to find anything from grid services log files.
            - Ticket # 221441: Could not find unique HPC input file on Trestles. Node was not able to access the file system.
            - Ticket # 223945: GridFTP transfer failure from Trestles gsiftp://trestles-dm1.sdsc.edu:2811/ endpoint. There was a transient issue. SDSC administrators were not able to replicate the issue next day.
            - Ticket # 222312: GRAM5 service on Trestles was loading an incorrect MPI module, causing jobs to fail. SDSC administrators

changed the GRAM service configuration scripts to fix the problem.
    - Investigated ways to support UltraScan on Stampede.
    - Assisted gateway PI on submitting renewal allocation application to April 2013 XRAC Committee.
    - Ultrascan Gateway PI Borries Demeler conducted a workshop in India sponsored by the Beckman Institute. The workshop presented XSEDE and XSEDE Science Gateways to the international biophysics community. IU ECSS personnel assisted in ensuring the workshop training sessions were monitored in real-time to guarantee a smooth user experience.
- ***Evaluation of Airavata with ADaM Toolkit***
  - Objectives: Assist the project team in using XSEDE resources to execute data mining applications through simpler gateway interfaces.
  - Detailed activities concluded during this reporting period include:
    - Job scheduling per node was developed. Users can schedule their workflow per node through submission of a single HTTP request to the middleware, rather than multiple requests to each application.
    - This quarter's effort also focused on integrating a gateway data management with Apache Airavata gateway middleware. The data registry will help catalog all executions performed on XSEDE resources. Current implementation has focused on the Ranger cluster, but transition to other XSEDE resources is in progress.
- ***Einstein Genome Gateway (science gateway)*** The ECSS project is now completed. The gateway requested the gateway hosting resources, which was fulfilled. Due to changes to the project team and re-architecture of the gateway middleware, the PI required no further assistance at this point.

Extended Support for Training, Education, and Outreach (WBS 1.5.3)

Type	Title	Location	Dates	Hours	Number of Participants	Number of *Under-represented persons	Method
Conference Talk/presentation /panel	Realizing the universe on XSEDE	ECSS Symposium	December 18th, 2012	0.5	20	1	Virtual
Conference Talk/presentation /panel	The Apache Software Foundation, Cyberinfrastructure, and Scientific Software: Beyond Open Source	SC12, Salt Lake City	November 13th, 2012	2	10	3	Synchronous

Conference Talk/presentation /panel	Open community software: Building science gateways and workflows	SC12, Salt Lake City	November 12-14th, 2012	1.5	20	3	Synchronous
Conference Talk/presentation /panel	Open community software: Building science gateways and workflows	JSMF Workshop, Bloomington, IN	November 16-17th, 2012	0.5	10	1	Synchronous
Conference Talk/presentation /panel	Building Scientific Workflows for the Geosciences with Open Community Software	American Geophysical Union, San Francisco	December 7th, 2012	0.5	25	5	Synchronous

Table 2. ECSS EOT Activities for Q4 of Calendar 2012. *Traditionally underrepresented groups.

Campus Bridging (WBS 1.6.5)

Discussion of campus bridging within XSEDE and within the national cyberinfrastructure community

In Q2 of PY2, the Campus Bridging team continued to disseminate information about XSEDE's Campus Bridging via videos produced in Q1PY2: https://pti.iu.edu/campusbridging/what-is-campus-bridging and https://pti.iu.edu/campusbridging/penguin-computing-and-iu. The bulk of Campus Bridging efforts were in the area of moving the GFFS Pilot project forward and in the software packaging projects. One report describing priorities for Campus Bridging in years 2-5 was published, and a detailed plan for cluster software distribution was drafted and disseminated within XSEDE for comment.

GFFS Pilot Project

GFFS Pilot teams met at SC12 in order to answer questions and get individual sites using the GFFS software, as well as to iron out final difficulties using the UVA testbed grid. Campus Bridging teams met with Operations multiple times in order to work through documentation and installation packages. Operations released installers for XSEDE GFFS during the week of 12/31/2012. Texas A&M will be the first pilot site to work with the GFFS software.

Campus Bridging Software Packages

The Campus Bridging team has, in concert with Operations and Software Development and Integration teams, put together a list of XSEDE software which is approved for inclusion in the XSEDE Campus Bridging Rocks Rolls and packaged software. Campus Bridging is working to establish milestones for the packaging of the software and a distribution mechanism for users. Campus Bridging continues to work with Operations, A&D, and SD&I to establish a plan for software packaging that pursues XSEDE's strategic goals for making XSEDE services available to campuses using the Campus Bridging software packages. The first phase of software packaging will focus on basic functionality and scientific software, while later phases will pursue tighter integration with XSEDE. Cornell will lead the packaging efforts, with volunteers at IU and SURA institutions to test software installation after Operations has tested installation functionality internally.

Challenges in Program Year Two

Campus Bridging anticipates challenges in reestablishing enthusiasm in the GFFS pilot sites for working with the software. Some of the sites have been reticent or critical of XSEDE due to the delays in pilot testing, and the Campus Bridging team will need to re-start the pilot process. Little time remains for software packages to be built, tested, documented and disseminated in PY2, and so the Campus Bridging team will need to pursue the software packaging efforts with alacrity in order to complete packaging initiatives before the end of the program year.

14.8 Publications

Conference Papers

Henschel, R., S. Simms, D. Hancock, S. Michael, T. Johnson, N. Heald, T. William, D. Berry, M. Allen, R. Knepper, et al., Demonstrating Lustre over a 100 Gbps Wide Area Network of 3500km, The International Conference for High Performance Computing, Network Storage, and Analysis (SC12), Dec 2012.

Husk, M. J., "Ink, Paper, Scissors: Experiments in Cutting Campus Printing Costs" SIGUCCS '12, Memphis, TN, ACM, Oct 2012.

Conference Proceedings

Henschel, R., S. Simms, D. Hancock, S. Michael, T. Johnson, N. Heald, T. William, D. Berry, M. Allen, R. Knepper, et al., " Demonstrating lustre over a 100Gbps wide area network of 3,500km" SC'12, Salt Lake City, Utah, Nov 2012.

Zhang, H., M. Boyles, and M. Ando, "3D-Time Series Analysis of Caries Lesion Activity for Oral Health Care" 2012 Workshop on Visual Analytics in Healthcare: Open Health Data held in conjunction with IEEE VisWeek 2012, Seattle, WA, Oct 2012.

Journal Article

Andrade, P., M. Babik, K. Bhaatt, P. Chand, D. Collados, V. Duggal, P. Feunte, S. Hayashi, E. Imamagic, P. Joshi, et al., "Distributed Monitoring Infrastructure for Worldwide LHC Computing Grid" Journal of Physics: Conference Series, vol. volume 396 Part 3, Dec 2012.

Gross, K., S. Hayashi, S. Tiege, and R. Quick, "Open Science Grid (OSG) Ticket Synchronization: Keeping Your Home Field Advantage In A Distributed Environment" Journal of Physics: Conference Series, vol. Volume 396, Part 6, Dec 2012.

Hayashi, S., S. Teige, and R. E. Quick, "The event notification and alarm system for the Open Science Grid operations center " Journal of Physics: Conference Series, no. Issue 3, Dec 2012.

Zhang, H., J. Weng, L. Jing, and Y. Zhong, "KnotPad: Visualizing and Exploring Knot Theory with Fluid Reidemeister Moves" Special Issue of IEEE Transactions on Visualization and Computer Graphics, Dec 2012.

Zhang, H., C. E. Frend, and M. J. Boyles, "Computer interfaces transform mathematical studies" SPIE Newsroom, no. Biomedical Optics & Medical Imaging, Oct 2012.

Presentation

Barnett, W. K., Business Intelligence in Translational Research: Research Networking as a Test Case, Educause 2012, http://www.educause.edu/annual-conference , Denver, CO, Nov 2012.

LeDuc, R. D., and W. K. Barnett, The National Center for Genome Analysis Support and Galaxy, IEEE/ACM Supercomputing (SC|12), OpenSFS.org booth, Nov 2012.

LeDuc, R., Experimental Design for NGS-Based Transcriptomics for Non_model Organisms, World Genome Data Summit, San Francisco, Nov 2012.

Miller, J., OpenSFS at Indiana University, Supercomputing 2012, Salt Lake City, Utah, Nov 2012.

Pierce, M., and S. Marru, JSMF Workshop on Plug-and-Play Macroscopes, Nov 2012.

Husk, M. J., Ink, Paper, Scissors: Experiments in Cutting Campus Printing Costs, SIGUCCS '12, Memphis, TN, Oct 2012.

Kallback-Rose, K., Indiana University Site Report, HPSS Users Forum 2012, HPSS Users Forum 2012, http://www-hpc.cea.fr/en/HUF2012/index.htm, Paris, France, Oct 2012.

LeDuc, R., Genomics, Transcriptomics, and Proteomics: Engaging Biologists, 8th IEEE International Conference on eScience 2012, Chicago, Illinois, Oct 2012.

Report

Simms, S., M. Davy, B. Hammond, M. R. Link, S. Teige, M. - H. Baik, Y. Manri, R. Lord, D. F. McMullen, J. C. Huffman, et al., Indiana University’s SC|07 Bandwidth Challenge award-winning project: Using the Data Capacitor for Remote Data Collection, Analysis, and Visualization , Nov 2012.

Stewart, C. A., T. M. Miller, D. Y. Hancock, S. Marru, M. E. Pierce, M. R. Link, S. C. Simms, K. Seiffert, J. Wernert, and J. Bolte, Indiana University Pervasive Technology Institute – Research Technologies: XSEDE Service Provider and XSEDE subcontract report (PY1: 1 July 2011 to 30 June 2012) , Oct 2012.

14.9 Metrics

14.9.1 Standard User Assistance Metrics

User Information and Interfaces (WBS 1.3.2)

Knowledge Base

Summary statistics for the XSEDE Knowledge Base:

Metric	For current quarter
Number of KB documents available at end of quarter	574
Number of new KB documents added	36
Total number of retrievals	219,363
Total number of retrievals minus bots	116,241

Table 3. High-level XSEDE Knowledge Base metrics for current quarter.

Metric	PY to date (when applicable)
Number of KB documents available at end of quarter	574
Number of new KB documents added	98
Total number of retrievals	393,575
Total number of retrievals minus bots	204,228

Table 4. High-level XSEDE Knowledge Base metrics for current period and project year to date.

Knowledge Base

Summary statistics for the XSEDE Knowledge Base:

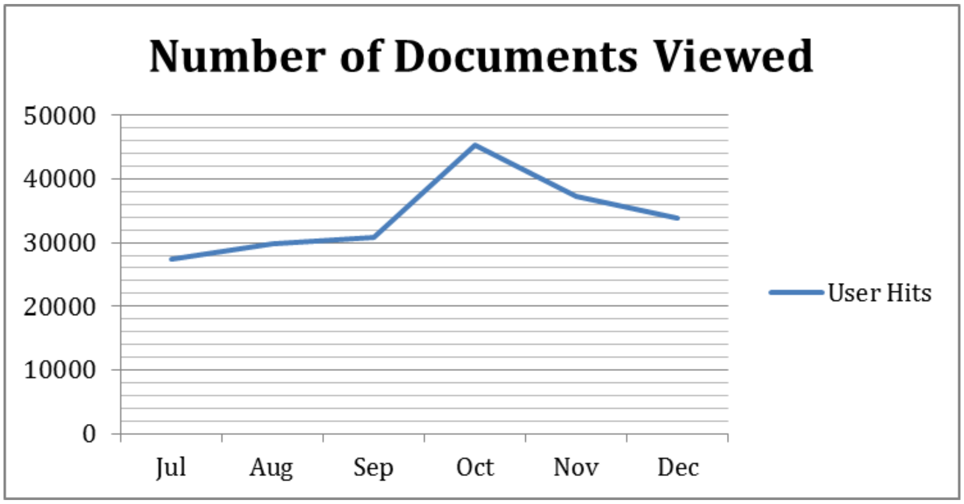


Figure 3. Total Knowledge Base accesses by month, current program year to date.

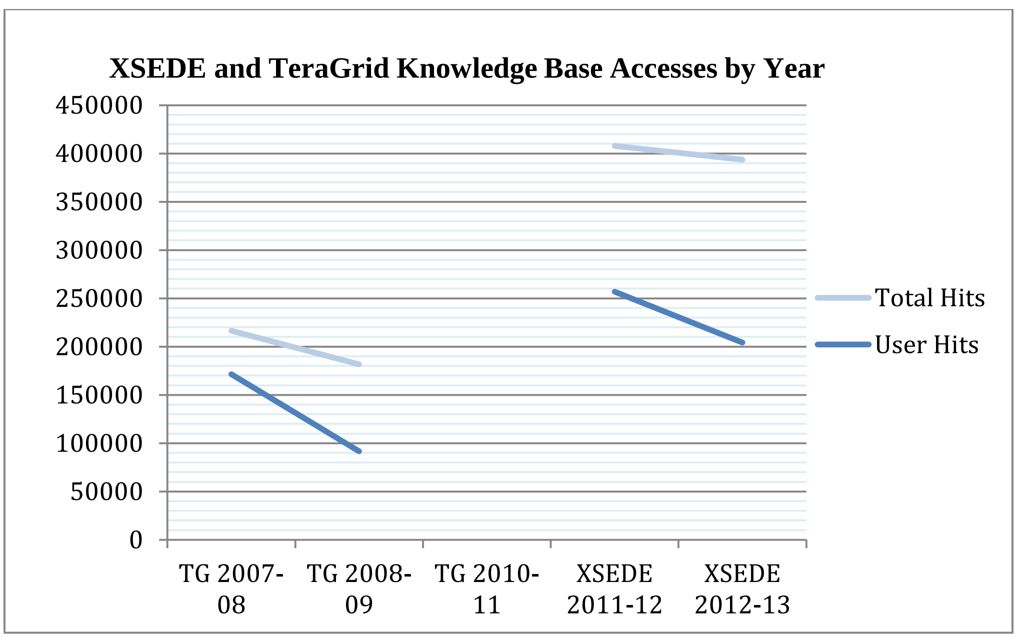


Figure 4. XSEDE and TeraGrid Knowledge Base annual accesses. (Data are unavailable for 2009/2010.)

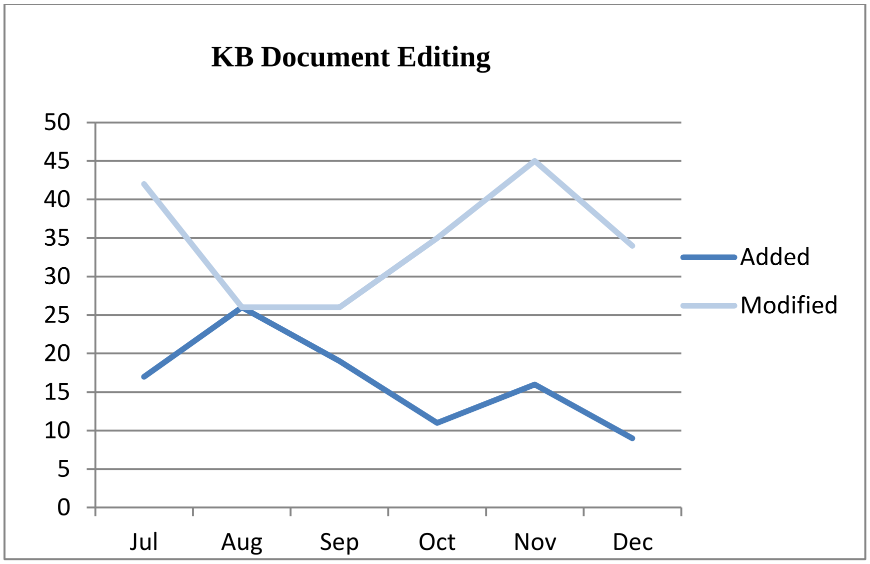


Figure 5. Knowledge Base editing activity (new entries added; existing entries modified or removed) by month, current program year to date.

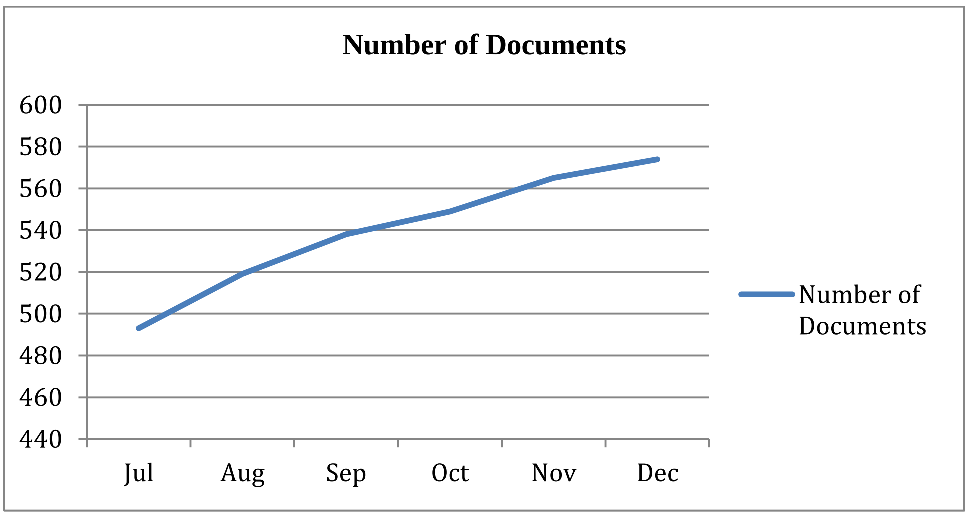


Figure 6. Total number of documents in XSEDE Knowledge Base by month, current program year to date.

14.9.2 SP-specific Metrics

14.9.2.1 Usage metrics – current quarter

	# Allocations	# VMs allocated	# TB allocated	System	Storage high water mark	TB written	TB read
Quarry VM	0	38					
Rockhopper				2,022			
Data Capacitor WAN	40		6.5	5.1B	322	125	96
Scholarly Data Archive – HPSS							

Table 5. Service Provider system key usage metrics for the current quarter (Q4 of 2012 –October-December 2012).

System	Overall % uptime	# planned downtimes	Planned downtime duration total (minutes)	# unplanned downtimes	Unplanned downtime duration total (minutes)	Total minutes in reporting period
Quarry VM	99.9%	1	15	2	1,400	132,480
Rockhopper	100%	0	0	0	0	129,600
Data Capacitor WAN	99.78	3	1,620	0	0	132,480
Scholarly Data Archive – HPSS						

Table 6. Service Provider system key usage metrics for the current quarter (Q4 of 2012 –October-December 2012).

14.9.2.2 Usage metrics – project year 2

System	# Allocations	# VMs allocated	# TB allocated	# accesses	Storage high water mark	TB written	TB read
Quarry VM	25	54					
Rockhopper				3,768			
Data Capacitor WAN	47		6.5	41.1B	322	260	305
Scholarly Data Archive – HPSS							

Table 7. Service Provider system key usage metrics for PY2 (July 2012–December 2012).

System	Overall % uptime	# planned downtimes	Planned downtime duration total (minutes)	# unplanned downtimes	Unplanned downtime duration total (minutes)	Total minutes in reporting period
Quarry VM	99.4	2	225	3	1,418	263,520
Rockhopper	100%	0	0	0	0	259,200
Data Capacitor WAN	99.28	4	1,860	1	52	264,960
Scholarly Data Archive – HPSS						

Table 8. Service Provider system key usage metrics for PY2 (July 2012–December 2012).

14.9.3 Standard systems metrics

N/A.

15 Georgia Tech - Service Provider Quarterly Report

15.1 Executive Summary

The Keeneland Project delivered XSEDE production on the Keeneland Initial Delivery System (KIDS) through December 2012 and began production on the Keeneland Full Scale System (KFS) at the end of October 2012. Both systems are focused on GPU-accelerated computing.

15.1.1 *Resource Description*

KIDS – 120-node cluster composed of HP SL390 nodes, each with two Westmere CPUs, three NVIDIA M2090 GPUs, 24 GB host memory, and a Mellanox QDR IB interconnect through a QLogic QDR IB enterprise switch.

KFS – 264-node cluster composed of HP SL250 nodes, each with two Sandy Bridge CPUs, three NVIDIA M2090 GPUs, 32 GB host memory, and a Mellanox FDR IB interconnect through a Mellanox FDR IB enterprise switch.

15.2 Science Highlights

The Keeneland systems XSEDE production has primarily been for chemistry, physics, and materials research.

- Understanding ion solvation at the air/water interface from adaptive QM/MM molecular dynamics simulations
- Evolution of Structure, Function, and Folding of RNA:Protein Complexes in Translation
- Computational Relativistic Astrophysics Models
- Testing universality in diblock copolymers using Graphics Processing Units

15.3 User-facing Activities

15.3.1 *System Activities*

The Keeneland Project made KIDS available to the XSEDE user community as a production resource until KFS became available. After KFS was available, most of the production workload was transitioned to KFS during November 2012, and the transition was completed in December. Development, discretionary accounts, and EOT activities remain on KIDS.

15.3.2 *Services Activities*

The Keeneland Project with partner UTK released new versions of MAGMA to take advantage of GPU acceleration.

15.4 Security

Nothing.

15.5 Education, Outreach, and Training Activities

Keeneland provided support for an SC12 tutorial and for the PSC OpenACC workshop.

Type	Title	Location	Date(s)	Hours	Number of Participants	Number of Under-represented people	Method
Hands-on Tutorial	Scalable Heterogeneous Computing on GPU Clusters	SC12, Salt Lake City, UT	11 Nov 2012	8	50		S
Workshop	OpenACC Workshop	GT, Atlanta, GA	15-16 Jan 2013	10	11		S

15.6 SP Collaborations

Keeneland collaborated with the Pittsburgh Supercomputing Center to provide the platform for the OpenACC Workshop and hosted a remote site at Georgia Tech.

15.7 SP-Specific Activities

Nothing.

15.8 Publications

- **CONFERENCES/PRESENTATIONS**

1. Full-day tutorial "Scalable Heterogeneous Computing on GPU Clusters" at SC12.
2. "Early Evaluation of Directive-Based GPU Programming Models for Productive Exascale Computing", at SC12.
3. The work on Ocelot/GPUs and on Shadowfax was presented at the CERCS IAB meeting to industry partners including HP, IBM, and Intel.
4. T. Dong, T. Kolev, R. Rieben, V. Dobrev, S. Tomov, and J. Dongarra, "Acceleration of the BLAST hydro code on GPUs", SC'12 Poster (available upon request).
5. A. Haidar, S. Tomov, J. Dongarra, R. Solca, and T. Schulthess, "A novel hybrid CPU-GPU generalized eigensolver for electronic structure calculations based on fine grained memory aware tasks", SC'12 Poster (available upon request).
6. "Matrices Over Runtime Systems @ Exascale", SC'12 Poster (available upon request).

- **PUBLICATIONS**

1. Seyong Lee, Jeffrey S. Vetter, "Early Evaluation of Directive-Based GPU Programming Models for Productive Exascale Computing", proceedings of SC12, 2012.
2. Karsten Schwan, "Fine-grained Resource Scheduling on High-Performance GPGPU Clusters" under submission to a first tier HPC conference (the rebuttal phase).

3. Peng Du, Stanimire Tomov, and Jack Dongarra, "Providing GPU capability to LU and QR within the ScaLAPACK framework", LAPACK Working Note 272 (also UTK CS Technical report UT-CS-12-699), September, 2012.
4. H. Anzt, S. Tomov, J. Dongarra, and V. Heuveline, "A Block-Asynchronous Relaxation Method for Graphics Processing Units", SIAM Journal on Scientific Computing (submitted on 10/15/2012, available upon request).

15.9 Metrics

Keeneland metrics were included with NICS metrics.

16 NICS - Service Provider Quarterly Report

16.1 Executive Summary

In 2009, the National Institute for Computational Sciences (NICS) delivered the first academic petaflop computer to the NSF community—a Cray XT5 called Kraken. By the end of 2010, systems at NICS were delivering more than 70% of all NSF compute cycles. This quarter, Kraken sustained a utilization of 96% and a 99% uptime while providing roughly 55% of the total CPU hours delivered by XSEDE resources (Table 12, Figure 42).

The addition of the SGI Altix, called Nautilus, and the Remote Data and Visualization (RDAV) center serves to broaden the services provided by NICS to the NSF community and increases the potential for breakthrough science (Section 16.2). RDAV's purpose is to aid in the significant challenge of transforming large-scale data into knowledge and insight by providing scientists with well-engineered and well-supported remote visualization, analysis, and scientific workflow technologies. Nautilus provided a 98% uptime for the quarter and 60% utilization.

Support staff at NICS responded to 758 new XSEDE tickets and closed 776 tickets (Table 14) during the quarter.

16.1.1 <u>*Resource Description*</u>

NICS currently has two NSF funded computational resources: Kraken and Nautilus. These systems share a Network File System (NFS) that contains user directories, project directories and software directories. One-time password tokens provide secure access to both the computational and storage resources at NICS.

16.1.1.1 Kraken

Kraken is a Cray XT5 consisting of 9,408 compute nodes, each containing two 6-core AMD Istanbul Opteron processors and 16 GB of on-node memory. The result is 112,896 compute cores that deliver 1.17 PF at peak performance with 147 TB total memory. Communications take place over the Cray SeaStar2+ interconnect. A parallel Lustre file system provides 3.3 PB (raw) of short-term data storage.

16.1.1.2 Nautilus

Nautilus, an SGI Altix UV 1000 system, is the centerpiece of NICS Remote Data and Visualization (RDAV) Center that is also located at ORNL. It has 1024 cores (Intel Nehalem EX processors), 4 TB of global shared memory, and 8 GPUs in a single system image yielding 8.2 TF at peak performance. A parallel Lustre file system provides 427 TB (raw) of short-term data storage.

16.1.1.3 HPSS Archival Storage

The High Performance Storage System (HPSS), developed and operated by ORNL, is capable of archiving hundreds of petabytes of data and can be accessed by all major leadership computing platforms. Incoming data is written to disk and later migrated to tape for long term archiving. This hierarchical infrastructure provides high-performance data transfers while leveraging cost effective tape technologies. Robotic tape libraries provide tape storage. The center has four SL8500 tape libraries holding up to 10,000 cartridges each. The libraries house a total of 24 T10K-A tape drives (500 GB cartridges, uncompressed), 60 T-10K-B tape drives (1 terabyte cartridges, uncompressed), and 20 T10K-C tape drives (5 terabyte cartridges, uncompressed). Each T10K-A and T10K-B drive has a bandwidth of 120 MB/s. Each T10K-C tape drive has a bandwidth of 240 MB/s. Disk storage is provided by DDN storage arrays with nearly a petabyte of capacity and over 12 GB/s of bandwidth. This infrastructure has allowed the archival system to scale to meet increasingly demanding capacity and bandwidth requirements with more than 12.4 PB of NICS data stored as of October 2012.

16.2 Science Highlights

16.2.1.1 Biophysics: Large-scale molecular dynamics simulations of anesthetic effects on ion channels (Pei Tang, University of Pittsburgh School of Medicine)

See main body of XSEDE quarterly report, 2.1.

16.2.1.2 Biochemistry: Evaluating and improving the performance of RNA force fields in molecular dynamics simulations (Thomas Cheatham, University of Utah College of Pharmacy)

See main body of XSEDE quarterly report, 2.2.

16.2.1.3 Biomass Research: Cellulase Enzyme Structure-Function Relationships (Gregg T. Beckham, National Renewable Energy Laboratory)

See main body of XSEDE quarterly report, 2.4.

16.2.1.4 Project aimed at exploring gap between data and information through unconventional visualization method wins jury prize at media festival

Collaborative work performed by the Remote Data Analysis and Visualization Center (RDAV) and University of Tennessee (UT), Knoxville, artist Evan Meaney that examines the interplay of data, information, and knowledge has won the jury prize for the Distributed Microtopias exhibition at the 15th Annual Finger Lakes Environmental Film Festival (FLEFF).

The RDAV–Meaney collaborative project, entitled “Null_Sets,” is a collection of artwork that visualizes the size and structure of data. The artwork was created using an open-source script developed at RDAV with which whole bodies of text, from classic literature to HTML to genomic data, can be exported as digital images.

“In a gallery, we can analyze these data sets side by side and consider the differences between, say, Moby Dick and an X-chromosome,” Szczepanski said. “Our method relies on an encoding that represents the changes in pixel color and intensity, and might be adapted to explore how values in a dataset change.”

“Null_Sets explores the gap between data and information,” Meaney said. “This project makes it possible to visualize both the size and architecture of large-scale data sets through an aesthetic lens.”

The novel use of encoding employed by Null_Sets coincides with the focus of this year’s FLEFF, the exploration of what it terms “Distributed Microtopias” and defines as projects that “run across distributed networks like the Internet to provoke and educate from remote locations on a sustainable scale, expand knowledge rather than contain it, invite participation and exploration, and unhinge familiar habits of thinking to envision new possibilities for historical and cultural clarity."

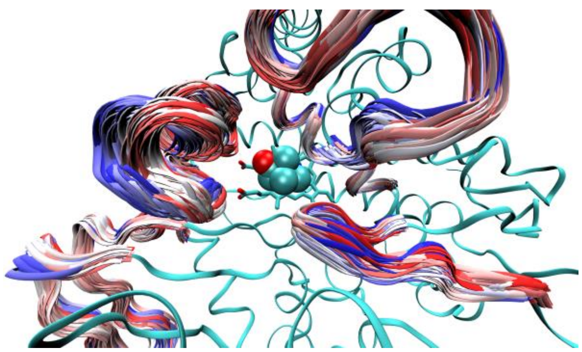
The project took shape in the spring of 2010 when Szczepanski, searching for digital media artists with whom RDAV could collaborate, contacted Meaney under the advice of UT's visual arts committee. After discussing Null_Sets and the theory behind it with Meaney, Szczepanski wrote the initial code, and then a student assumed the task. As project designer and director, Meaney suggested revisions to the code to improve the work, chose the texts, handled tasks related to producing physical images, made submissions to shows and festivals, and printed catalogs, Szczepanski said. "The techniques we developed in this project laid the groundwork for a larger project that will likely use the Nautilus supercomputer in the future," she said.

16.2.1.5 *Biochemistry: Three Professors Combine neutrons with Superconducting Magnet and Supercomputing to Probe Enzyme Function*

OAK RIDGE, Tenn.—A team of three professors at the University of Tennessee, Knoxville (UTK), has combined high-tech experiments with supercomputing to probe the function of critical enzymes.

Jeremy Smith, Nitin Jain, and Jerome Baudry of the Department of Biochemistry and Cellular and Molecular Biology recently applied the experimental technologies of neutron scattering at ORNL and nuclear magnetic resonance (NMR) spectroscopy at UTK in concert with molecular dynamics (MD) supercomputer simulations involving the NICS Kraken supercomputer to gain an in-depth understanding of motions in cytochrome P450.

Cytochrome P450s are highly effective biocatalysts present in almost all higher organisms. In humans, they increase the rate of chemical reactions involved in the processing of drugs, formation of fats and steroids, development of cancerous cells, and breaking down of pollutants.



Research revealed the dynamic changes that take place in the enzyme cytochrome P450 upon substrate binding.

Cytochrome P450s are inherently very flexible enzymes and this flexibility is key in how they metabolize a multitude of foreign chemicals such as drugs. Understanding the various internal motions these enzymes undergo to bind different drugs will aid in the design of medicines. This is because drug designers will be able to predict how specific drug candidates will interact with these enzymes and whether they will eventually fail due to chemical interaction with P450s in the patients' cells.

This research required collaboration between the three laboratories, each with its own expertise in one of three respective areas: neutron scattering, NMR, and computer simulations. Such an integration was necessary to obtain a detailed picture of the motional dance P450s undergo to achieve binding to a target. The results of their study will soon be published in Biophysical Journal as "Coupled Flexibility Change in Cytochrome P450cam Substrate Binding Determined by Neutron Scattering, NMR and Molecular Dynamics Simulation."

“The question of how flexible P450s are and how that relates to their function has long puzzled scientists in the drug metabolism area,” Jain said.“ Being able to demonstrate and utilize the complementary nature of the three technologies to address this important question in one P450 now opens up doors to study dynamic aspects of other human drug-binding P450s, with enormous potential in application to drug design.”

“The work involving the three UTK professors illustrates how modern research has become highly collaborative, with each faculty member bringing specific expertise integrated into finding a specific solution,” Smith said. “Also, it illustrates how major local facilities such as supercomputing and neutron sources can be combined for the performance of leading-edge research.”

The neutron scattering experiments were conducted using the BASIS and CNCS instruments at the Spallation Neutron Source at ORNL and the HFBS instrument at the National Institute of Standards and Technology (NIST). Assistance was provided by Eugene Mamontov of ORNL with BASIS, George Ehlers of ORNL with CNCS, and Madhu Tyagi of NIST with HFBS. Liang Hong and Nikolai Smolin of the UT/ORNL Center for Molecular Biophysics provided code for analysis and discussions.

NMR experiments were carried out at the high-field NMR facility of UTK, which operates a NMR spectrometer with a 600 MHz superconducting magnet. NMR is a technique that allows scientists to look at molecules very much like its sibling technique MRI, or magnetic resonance imaging, allows physicians to see the internal structures of the human body.

For the MD computer simulations, the research team employed the Kraken, Franklin, and Hopper supercomputers. Kraken, which is managed by NICS for the National Science Foundation (NSF), is a Cray XT5 capable of more than a petaflop—a thousand trillion calculations per second.

The professors’ research team is composed of Yinglong Miao, Zheng Yi, Carey Cantrell of UTK’s Department of Biochemistry and Cellular and Molecular Biology; and Dennis Glass of the UT Graduate School of Genome Science and Technology. All of the researchers except for Cantrell and Jain are also affiliated with the UT/ORNL Center for Molecular Biophysics. A NSF award supported this research project.

16.3 User-facing Activities

16.3.1 System Activities

16.3.1.1 Kraken

Availability

Kraken had an overall system availability of 99% for this quarter with 27 total hours of downtime. Downtime for the quarter consisted of 6 hours of scheduled downtime and 18 hours of unscheduled downtime (Table 1).

Table 12: Summary of maintenance Stats for Kraken in Q2PY2.

Maintenance Stats -- Kraken Cray XT5	
Number of planned reboots	2
Number of unplanned reboots	12
Total reboots	14
Job failures due to system faults	3325
Total time in period	2209 hrs (100%)
Scheduled Downtime	6 hours (1%)
Unscheduled Downtime	18 hours (1%)
Total Downtime	27 hours (1%)
Total time available to users (total-downtime)	2182 hours (99%)
% System Utilization	96%

16.3.1.2 Nautilus

Availability

Nautilus had an overall system availability of 98% for this quarter. Downtime for the quarter consisted of 44.5 hours of scheduled downtime and 1 hour of unscheduled downtime (Table 2).

Table 13: Summary of maintenance Stats for Nautilus in Q2PY2.

Maintenance Stats -- Nautilus SGI UV1000	
Number of planned reboots	6
Number of unplanned reboots	1
Total reboots	7
Total time in period	2209 hrs (100%)
Scheduled Downtime	44.5 hours (2%)
Unscheduled Downtime	1 hours (0%)
Total Downtime	45.5 hours (2%)
Total time available to users (total-downtime)	2164 hours (98%)
% System Utilization	60%

16.3.2 Services Activities

16.3.2.1 Kraken

Software Packages
NICS currently supports 407 unique application builds on Kraken that include pre-compiled binaries and builds with PGI, GNU, Cray, and Intel compilers. These builds include 207 unique versions and 130 unique applications and libraries.

Environment
In October 2012, a portals patch was applied on Kraken to fix a bug that was causing occasional job failures. The symptoms of the bug were that a job would fail to fully launch and hang until killed by the user, systems staff, or the scheduler at the wall clock limit. Significant effort went into isolating and understanding this bug. Once isolated, Cray needed time to develop and test the patch. Since this patch has been installed there have been no confirmed occurrences of this bug.

16.3.2.2 Nautilus

Software Packages
NICS' staff currently supports 399 unique application builds on Nautilus that include pre-compiled binaries and builds with PGI, GNU, and Intel compilers. These builds include 218 unique versions and 117 unique applications and libraries.

Environment
In the last quarter, RDAV stood up an expansion to the capabilities provided by the Nautilus system. We rolled out four SGI UV10s, integrated with Nautilus and the shared Lustre file system, for users who wish to have dedicated hardware at their disposal. These UV10 systems, named "harpoon" nodes, each have 32 Intel Nehalem EX cores, 128 GB of memory, and an NVIDIA Tesla GPU. They are intended for users who are working to scale up their analysis and visualization and are not yet ready for the full Nautilus UV1000 system. In addition, they also have allowed us to deploy the final 8 NVIDIA GPUs for our center.

16.4 Security

No security incidents occurred at NICS during the quarter. In October 2012, NICS completed an internal security assessment based on NIST Special Publication 800-53, "Recommended Security Controls for Federal Information Systems and Organizations."

16.5 Education, Outreach, and Training Activities

Type	Title	Location	Hours	Date(s)	Number of Participants	Underrepresented Community
College Class, mentorship	Communicating Science with Video (Art Dept., UT-Knoxville)	Knoxville, TN	12	10/1 – 12/5	8	5
College Class guest lectures, INSC 584 and INSC 590	"College Algebra at the University of Tennessee: Understanding the students and their progress"	Knoxville, TN and webcast to remote locations	2	11/27	~80	unknown

Presentation	“NICS - Who we are and where you may fit in”	Knoxville, TN	1	11/29	15	unknown
Conference Exhibit	University of Tennessee research booth - SC12	Salt Lake City, Utah	23	11/12-15	~10000	unknown
Presentation	"Intel Xeon Phi: Experiences at NICS”	Salt Lake City, Utah: SC12	1	11/13	20	unknown
Presentation	"Beacon: A Path to Energy Efficient HPC"	Salt Lake City, Utah: SC12	1	11/14	20	unknown
Demonstration	"Applications Acceleration with the Intel Xeon Phi"	Salt Lake City, Utah: SC12	12	11/12-15	~200	unknown
Poster	“GenASiS: An Object-Oriented Approach to High Performance Multiphysics Code with Fortran 2003”	Salt Lake City, Utah: SC12	2	11/13	50	unknown
Poster	“Interface for Performance Environment Autoconfiguration Framework”	Salt Lake City, Utah: SC12	2	11/13	50	unknown
Presentation	“Application Accelerators in Computational Science: Challenges and Opportunities”	Salt Lake City, Utah: SC12	2	11/15	25	unknown
Poster	“Statistical Performance Analysis with HPCC”	Las Vegas, NV: Analytics 2012	2	10/8-9	40	unknown
Poster	“A Bayesian Approach for Workload Analysis and Modeling”	Las Vegas, NV: Analytics 2012	2	10/8-9	40	unknown

16.6 SP Collaborations

EPSCOR

The Experimental Program to Stimulate Competitive Research, or EPSCoR, establishes partnerships with government, higher education and industry that are designed to effect lasting improvements in a state's or region's research infrastructure, R&D capacity and hence, its national R&D competitiveness. NICS participates along with researchers from twenty-seven other states and the Commonwealth of Puerto Rico. The partnership is based on existing and planned collaborations in the advanced materials and systems biology domains where computational science is driving new approaches and insights. The collaborative team has proposed to build cyberinfrastructure (CI) linked, community specific knowledge environments that embody the desktop to XSEDE ecosystem by using campus-based CI at a regional research institution as an essential bridge for connecting faculty investigators to national resources such as the XSEDE.

In Q2PY2 NICS EPSCoR staff generated new modules for HMMER for the latest upgrade on Kraken and began working on Systems Biology Science Gateway with the web interface known as PoPLAR: the Portal for Petascale Lifescience Applications and Research, currently can run BLAST and HMMER through portal and is still under testing for transferring large files for analysis. Staff also engaged with researchers from Medical University of South Carolina to use AutoDock on Kraken. In addition, Bhanu Rekepalli collaborated with Nick Panasik from Claflin University to port the LINUS python package to Kraken and with William Mondy on biocad modeling on Nautilus.

Keeneland

Keeneland is a five-year, $12 million NSF Track 2D award made to the Georgia Institute of Technology. The Keeneland goal is to make an experimental, high-performance computing system consisting of an HP system with NVIDIA Fermi accelerators available for use by the XSEDE user community. System support and user support are provided by NICS. Staff at Georgia Tech and Oak Ridge National Lab (ORNL) provides advanced application-support. Software development activities are funded at Georgia Tech, University of Tennessee, and ORNL.

The Keeneland project team has used the Keeneland Initial Delivery System (KIDS) to develop scientific libraries and programming tools to facilitate the development of science and engineering research applications and to provide a resource for early adopters to port codes and improve code performance.

In the most recent quarter, the larger final Keeneland system was moved into production. It was #75 on the November 2012 Top500 list. Allocations were awarded at recent XRAC meetings. Some allocations were moved from the Forge system at NCSA. The final Keeneland system will be operated as an XSEDE resource for the next two years. The Keeneland Initial Delivery System will also be used as an XSEDE resource devoted to classroom projects, workshops, and other special activities.

NCSA Blue Waters Project

The National Institute for Computational Sciences (NICS) staff has collaborated with the National Center for Supercomputing Applications (NCSA) Blue Waters project starting in January 2012 to facilitate and assist with the configuration and deployment of the Cray XE/XK system. This effort is focused on application support and system management. The NICS team has contributed to the project by the sharing of experience and information via discussions and presentations. Additionally, NICS has assisted with system monitoring and application work in preparation for acceptance tests.

NICS staff is actively collaborating on one PRAC support project with NCSA staff members. Additionally, NICS has provided assistance with the installation, maintenance, and utilization of a software/library tracking solution. Throughout the quarter four applications/benchmarks were ported and tested to meet Blue Waters acceptance test items.

Joint Institute for Computational Sciences

The University of Tennessee (UT) and Oak Ridge National Laboratory (ORNL) established the Joint Institute for Computational Sciences (JICS) in 1991 to encourage and facilitate the use of high performance computing in the state of Tennessee. JICS advances scientific discovery and state-of-the-art engineering by taking full advantage of the petascale computers supported by DOE and NSF and housed at ORNL facilities by enhancing knowledge of computational modeling and simulation through educating a new generation of scientists and engineers well versed in the application of computational modeling and simulation to solving the world's most challenging scientific and engineering problems.

JICS is staffed by joint faculty who hold dual appointments as faculty members in departments at UT and as staff members in ORNL research groups. The institute also employs professional research staff, postdoctoral fellows and students, and administrative staff. The JICS facility represents an investment by the state of Tennessee and features a state-of-the art interactive distance learning center auditorium with seating for 66 people, conference rooms, informal and open meeting space, executive offices for distinguished scientists and directors, and incubator suites for students and visiting staff.

The JICS facility is a hub of computational and engineering interactions. Joint faculty, postdocs, students, and research staff share the building, which is designed specifically to provide intellectual stimulation and interaction. The auditorium serves as the venue for invited lectures and seminars by representatives from academia, industry, and other laboratories, and the open lobby doubles as casual meeting space and functions as a site for informal presentations and poster sessions, including an annual 100+ student poster session.

16.7 SP-Specific Activities

AACE

In 2011 the Joint Institute for Computational Sciences (JICS) established the Application Acceleration Center of Excellence (AACE) in partnership with NICS, industry leading vendors, and academic institutions. The center's objectives are:

- Accelerate NSF projects toward exascale with state-of-the-art heterogeneous architectures
- Spur development of new algorithms and codes optimized for accelerator-based architectures
- Disseminate fundamental knowledge
- Facilitate effective exchange of expertise and cross-disciplinary collaboration

NICS is assisting NSF users with their transition to the Intel MIC architecture by researching parallelization techniques on the Intel MIC platform and by porting key NSF applications (already millions of lines of code) to the Intel MIC architecture in advance of its commercial release. NICS will also offer training on the Intel MIC architecture following its commercial debut.

"NICS has provided insight to Intel regarding the technology requirements of the scientific computing community," added Joe Curley, director of marketing for Intel's Technical Computing Group. "The impact of our partnership can be seen in the focus of our Intel MIC 'Knights Ferry' software development platform on extending well understood, high-level, standard programming languages and models."

NICS continues to engage a variety of technology providers to determine the role their technologies will play in the quest for exascale, while at the same time providing valued input for product development to meet the needs of the NSF research community.

Industrial Partnerships
NICS currently provides expertise and computational resources to three industrial partners. The goal of the partnerships is to speed innovations to market through application of leading edge simulation capabilities. The benefit to the industrial partners is a condensed design cycle and reduced prototyping and manufacturing costs.

16.8 Publications

16.8.1 User Publications

Submitted

1. Cardillo J., Chen Y., Newman J., Araya G., Jansen K. and Castillo L., DNS of turbulent boundary layers with surface roughness, under review in the J. of Fluid Mechanics, 2012.
2. F. X. Vázquez, V. M. Unger, and G. A. Voth, "Autoinhibition of Endophilin in Solution via Inter-domain Interactions", Biophys. J. (submitted).
3. H. Cui, C. Mim, E. Lyman, V. M. Unger, and G. A. Voth, "Understanding the Role of Amphipathic Helices in N-BAR Domain Driven Membrane Remodeling", Biophys. J. (submitted).
4. M. Simunovic, A. Srivastava, and G. A. Voth, "Linear Aggregation of Proteins on the Membrane: A Prelude to Endocytosis", Nature Communications (submitted).
5. J. Fan, M. G. Saunders, E. J. Haddadian, K. F. Freed, E. M. De La Cruz, and G. A. Voth, "Molecular Origins of Cofilin-linked Changes in Actin Filament Mechanics", J. Mol. Biol. (submitted).
6. A. V. Sinitskiy and G. A. Voth, "Coarse-Graining of Proteins Based on Elastic Network Models", Chem. Phys. (submitted).

Accepted

1. A. S. Schneider, C. J. Horowitz, J. Hughto and D. K. Berry, "The carbon-oxygen phase diagram of plasma mixtures in white dwarf stars", Journal of Physics Conference Series, in press 2012.
2. Dodd M., Ferrante A. "DNS of particle dispersion in a spatially developing turbulent boundary layer". International Conference on Multiphase Flow, Jeju, Korea, May 26-31, 2013.
3. Dodd M., Ferrante A. " A coupled pressure-correction/volume of fluid method for DNS of droplet-laden isotropic turbulence ," International Conference on Multiphase Flow, Jeju, Korea, May 26-31, 2013.
4. Shenoy, S., H. Nanda, and M. Lösche, "Membrane Association of the PTEN Tumor Suppressor: Electrostatic Interaction with Phosphatidylserine-Containing Bilayers and Regulatory Role of the C-Terminal Tail", J Struct Biol, 2012.

Published

1. M. Luisier, “Atomistic modeling of anharmonic phonon-phonon scattering in nanowires”, Phys. Rev. B 86, 245407 (2012).
2. J. Hughto, C. J. Horowitz, A. S. Schneider, Zach Medin, Andrew Cumming, "Direct MD simulation of liquid-solid phase equilibria for three-component plasma", Phys. Rev. E 86, 66413 (2012).
3. Grinberg, L., Deng, M., Lei, H., Insley, J.A., and Karniadakis, G.E. "Multiscale simulations of blood-flow: from a platelet to an artery". In Proceedings of XSEDE 2012: Chicago, IL, July 16-20, 2012. Article Number 33. ACM, New York, 2012.
4. Jagannathan, S. and Donzis, D. "Massively Parallel Direct Numerical Simulations of Forced Compressible Turbulence: a Hybrid MPI/OpenMP approach". In Proceedings of XSEDE 2012: Chicago, IL, July 16-20, 2012. ACM, New York, 2012.
5. Baraldi A. & Ferrante A. "DNS of fully-resolved droplet-laden isotropic turbulence: a mass-conserving volume of fluid method". In Proceedings of 23rd International Conference of Theoretical and Applied Mechanics (ICTAM: Beijing, China, August 19-24, 2012.
6. Baraldi A. & Ferrante A. "A VoF method for DNS of droplet-laden incompressible turbulence". 7th International Conference on Computational Fluid Dynamics: Big Island, Hawaii, July 9-13, 2012.
7. Dodd M., Webster K. & Ferrante A. "DNS of particle dispersion in a spatially developing turbulent boundary layer": 7th International Conference on Computational Fluid Dynamics: Big Island, Hawaii, July 9-13, 2012.
8. Diaz, M. A.; Zettergren, M.; Semeter, J. L.; Oppenheim, M., “Plasma parameter analysis of the Langmuir decay process via Particle-in-Cell simulations”, Annales Geophysicae, Volume 30, Issue 8, 2012, pp.1169-1183 (COPERNIUS Homepage), 10.5194/angeo-30-1169-2012.
9. Dimant, Yakov; Tambouret, Yann; Oppenheim, Meers, “Kinetic simulations of meter-scale structures in Convective Equatorial Ionospheric Storms (Spread-F)”, American Physical Society, 53rd Annual Meeting of the APS Division of Plasma Physics, November 14-18, 2011, abstract #UP9.087, 2011APS..DPPUP9087D.
10. Shenoy, S., H. Nanda, and M. Lösche, “Membrane Association of the PTEN Tumor Suppressor: Electrostatic Interaction with Phosphatidylserine-Containing Bilayers and Regulatory Role of the C-Terminal Tail”, J Struct Biol, 2012.
11. Dimant, Yakov; Oppenheim, Meers, “Macroscopic effects of E-region turbulence: Anomalous plasma heating and conductivity”, American Physical Society, 53rd Annual Meeting of the APS Division of Plasma Physics, November 14-18, 2011, abstract #CM1.000, 2011APS..DPPC10001D.
12. Pan, JJ, Chen, Q, Willenbring, D, Yoshida, K, Tillman, T, Kashlan, OB, Cohen, A, Kong, XP, Xu, Y, & Tang, P., “Structure of ELIC Co-crystallized with Its Competitive Antagonist Acetylcholine, Nature Communications”, PMC3316889, file://localhost/DOI/10.1038:ncomms1703, 2012.
13. Tillman T, Cheng MH, Chen Q, Tang P, Xu Y, “Reversal of ion charge selectivity renders the pentameric ligand-gated ion channel GLIC insensitive to anesthetics”, Biochemical J, in press (2012).
14. A. Li, K.F. Liu, A. Alexandru, “Critical point of $N\_f = 3$ QCD from lattice simulations in the canonical ensemble”, Phys. Rev., D84 (2011) 071503, [arXiv:1103.3045].

15. K.F. Liu, "Charge-dependent Azimuthal Correlations in Relativistic Heavy Ion Collisions and Electromagnetic Effects", Phys. Rev. C85 (2012) 014909, [arXiv:1109.4883].
16. H.W. Lin and K.F. Liu, "Comment on `Controversy concerning the definition of quark and gluon it angular momentum", Phys. Rev. D85 (2012) 058901, [arXiv:1111.0678].
17. Y. Yang, Y. Chen, G. Li, and K.F. Liu, "1^{-+} Meson a Hybrid?", [arXiv:1202.2205].
18. M. Lujan, A. Alexandru, T. Draper, W. Freeman, M. Gong, F.X. Lee, A. Li, K.F. Liu, N. Mathur, "The Delta_mix parameter in the overlap on domain-wall mixed action", Phys. Rev. D86 (2012) 014501, [arXiv:1204.6256].
19. K.F. Liu, W.C. Chang, H.Y. Cheng, and J.C. Peng, "Connected Sea Partons", [arXiv:1206.4339].
20. M. Gong, A. Li, A. Alexandru, Y. Chen, T. Draper, K.F. Liu, "Study of the scalar charmed-strange meson D_s0^* (2317) with chiral fermions", PoS LATTICE2010 (2010) 106, [arXiv:1103.0589].
21. K.F. Liu, M. Deka, T. Doi, Y.B. Yang, B. Chakraborty, Y. Chen, S.J. Dong, T. Draper, M. Gong, H.W. Lin et al., "Quark and Glue Momenta and Angular Momenta in the Proton --- a Lattice Calculation", PoS LATTICE2011 (2011) 164, [arXiv:1203.6388].
22. M. Gong, A. Li, A. Alexandru, T. Draper, K.F. Liu, "The Strangeness and Charmness of Nucleon from Overlap Fermions", PoS LATTICE2011 (2011) 156, [arXiv:1204.0685].
23. T. Hu, J. Huang, D. Li, K.F. Liu, B. Qin, J. Yang, L. Yang, "Development of 12kW RF Power Supply for CYCHU-10 Cyclotron", Conf. Proc. C1205201 (2012) 3416-3418.
24. K.F. Liu, "Research of Thermal Deformation on a Compact Cyclotron CYCHU-10", Conf. Proc. C110904 (2011) 1753-1755.

16.8.2 Staff Publications

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16.9 Metrics

16.9.1 Standard systems metrics

The following subsections contain system metrics for NICS’ resources that are allocated through XSEDE: Kraken and Nautilus.

Note that job wait times and job expansion factors as reported by XDMoD are skewed by user specified job dependencies. NICS has implemented an “effective queue time” metric to eliminate the influence of job dependencies on these statistics. The effective queue time is a measure of the wait time incurred only once a job is eligible to run and is not a factor of individual workflows. In the future job wait times and expansion factors will be reported based on effective queue times.

Another issue with wait time and expansion factor by job size, as currently reported, is that the job size bins overlap multiple scheduling queues at NICS, and thereby, overlap multiple scheduling policies. This too will be corrected in future reporting. Also note that the error bars associated with the mean values in Figure 19, Figure 20, Figure 28 and Figure 29 represent the standard deviation of the sampled mean which is the standard deviation divided by the square root of N, where N is the sample size.

16.9.2 Kraken

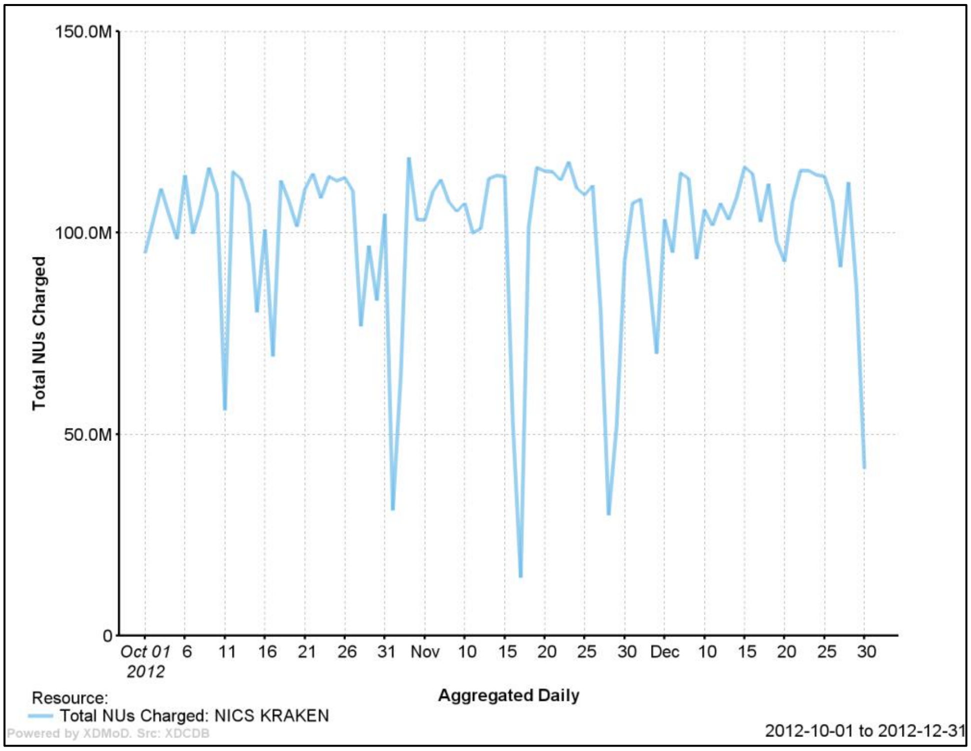


Figure 17: Daily resource consumption in Mega-normalized units ($1e^6$) charged on Kraken for Q2PY2.

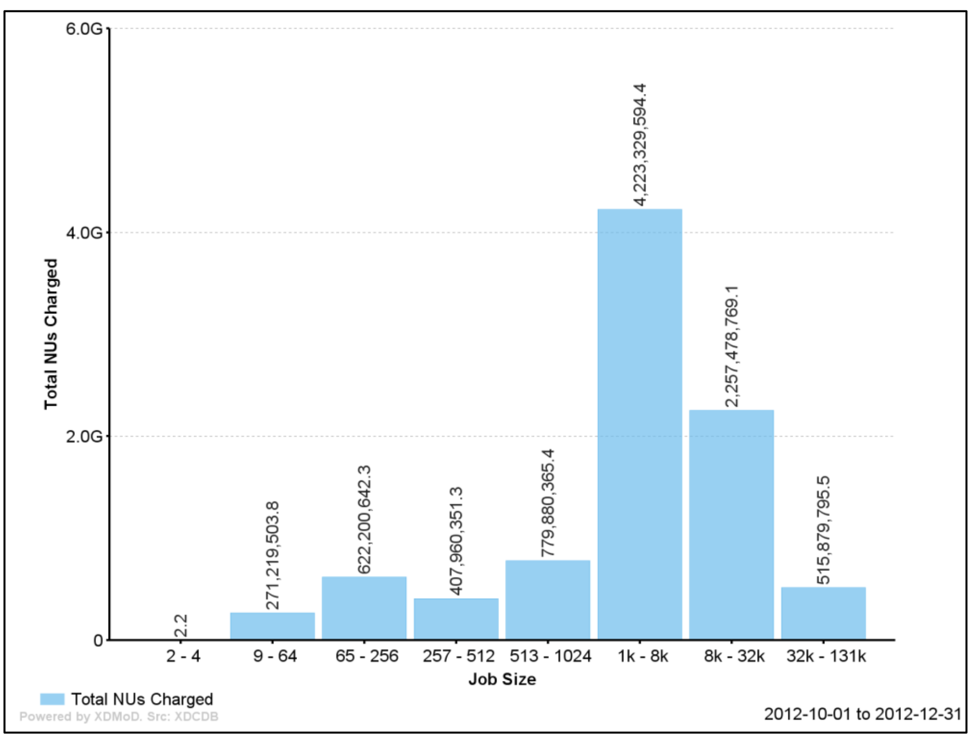


Figure 18: Total resource consumption in Giga-normalized units ($1e^9$) by job size for Kraken in Q2PY2.

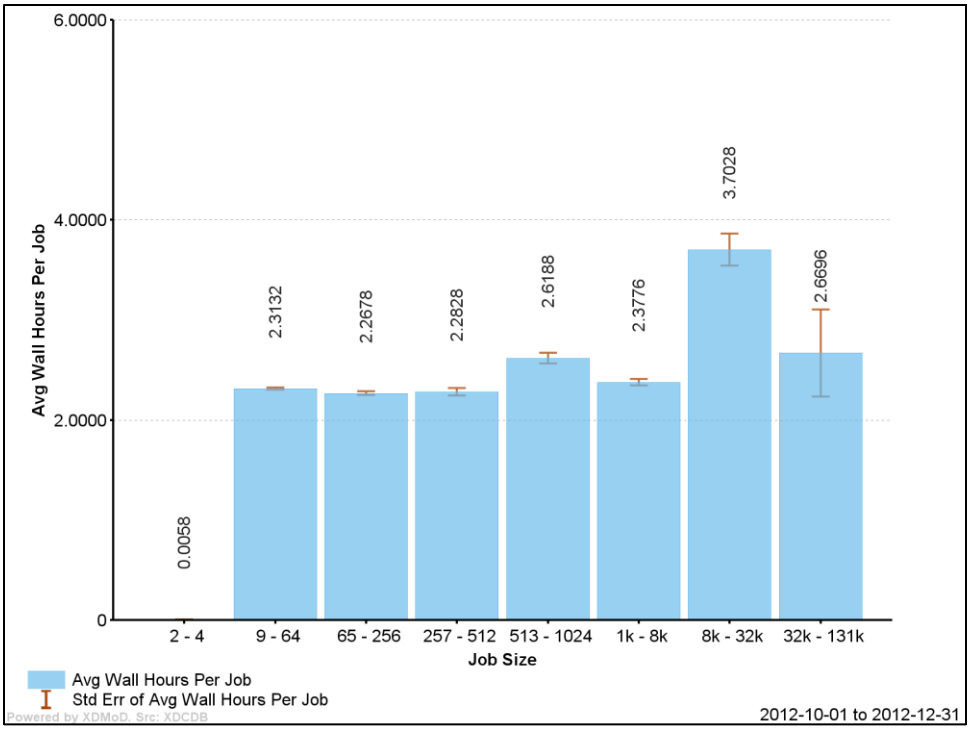


Figure 19: Average wall hours by job size on Kraken in Q2PY2.

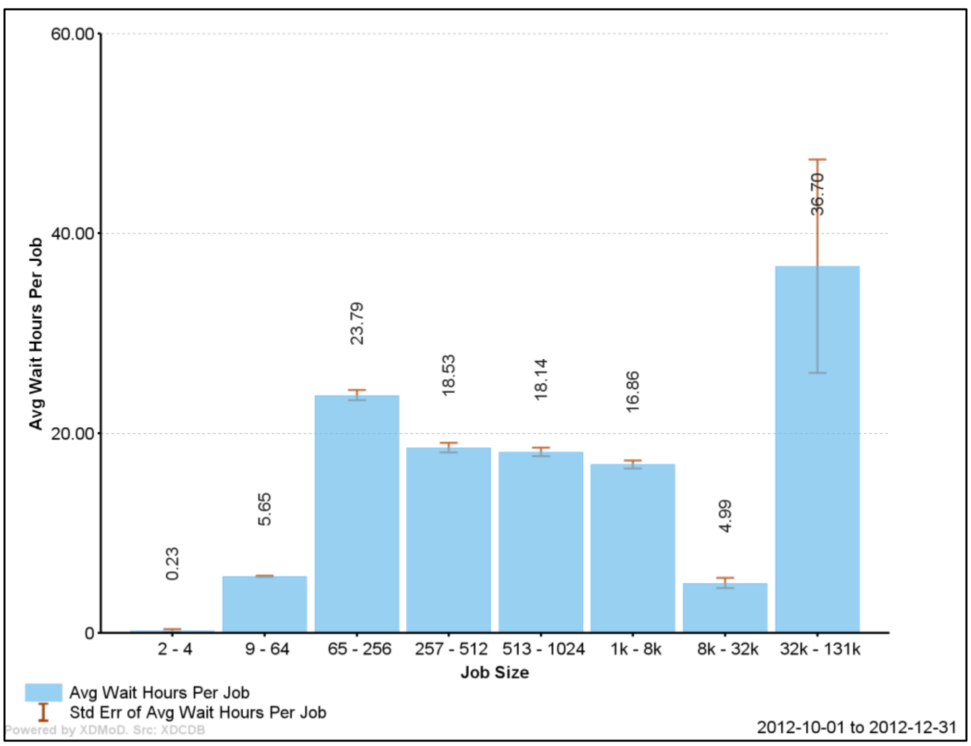


Figure 20: Average wait hours by job size on Kraken in Q2PY2.

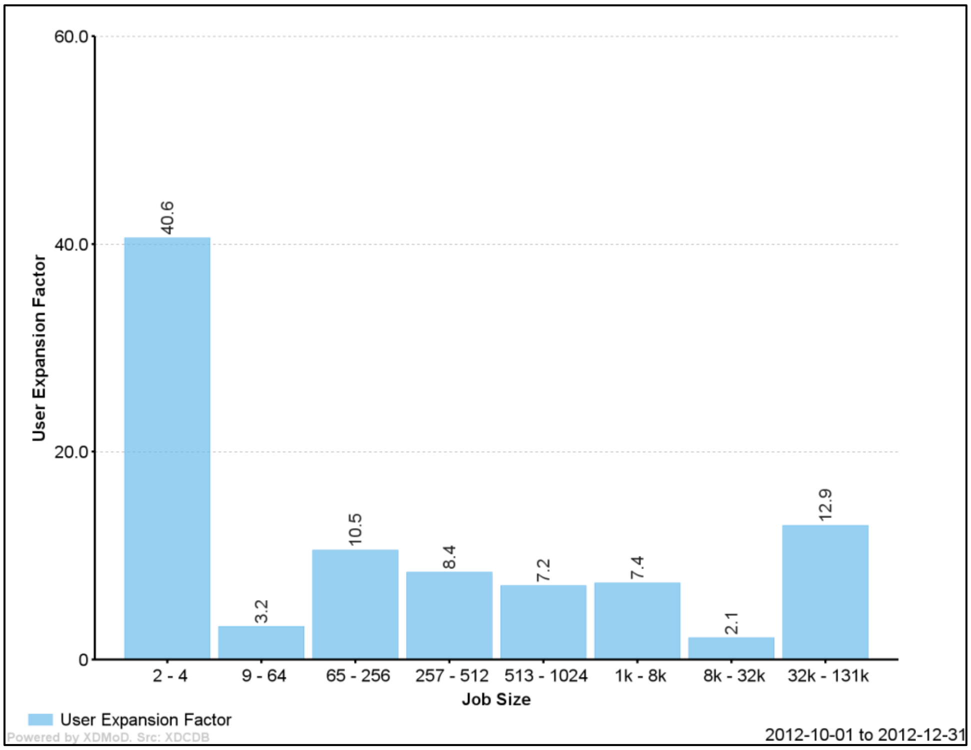


Figure 21: Expansion factor by job size for Kraken in Q2PY2.

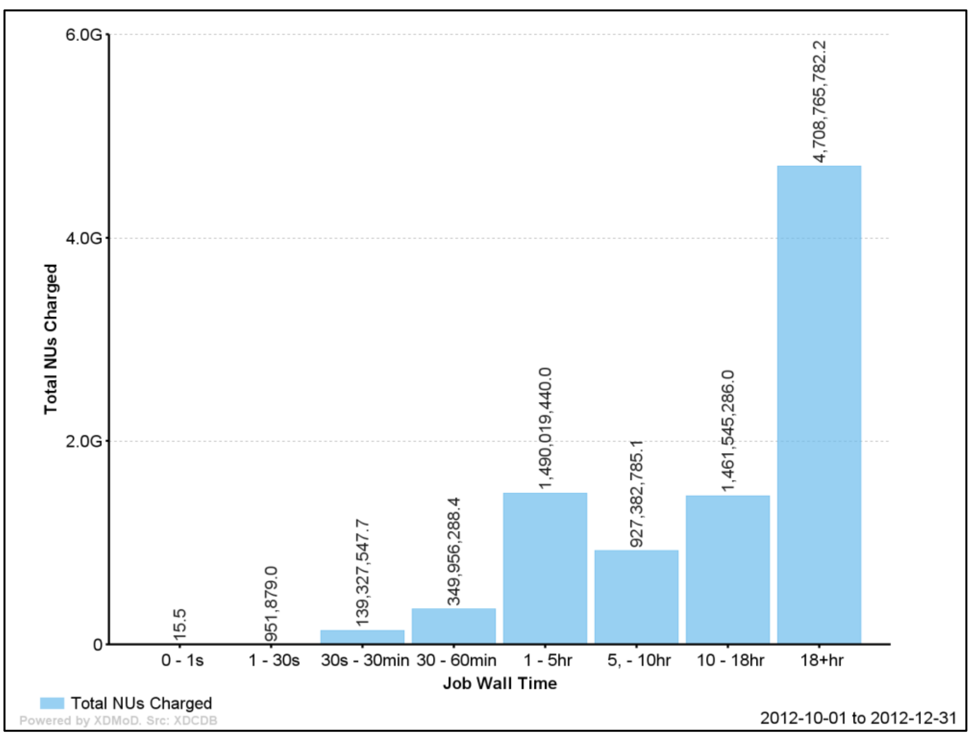


Figure 22: Total resource consumption in Giga-normalized units ($1e^9$) by wall time for Kraken in Q2PY2.

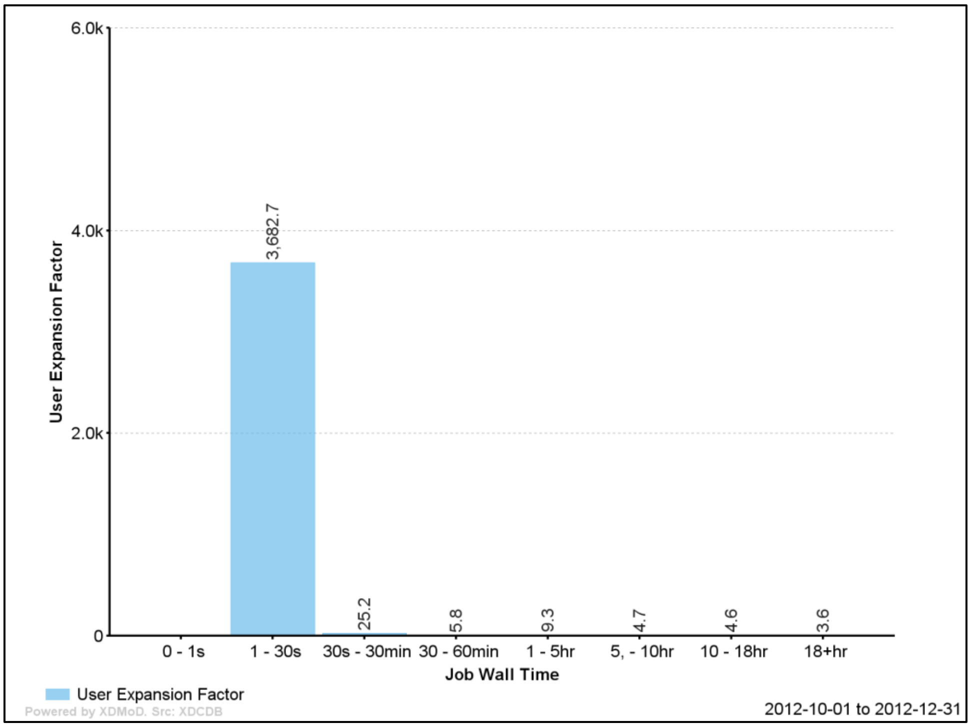


Figure 23: Resource consumption in mega-normalized units ($1e^6$) by field of science for Kraken in Q2PY2.

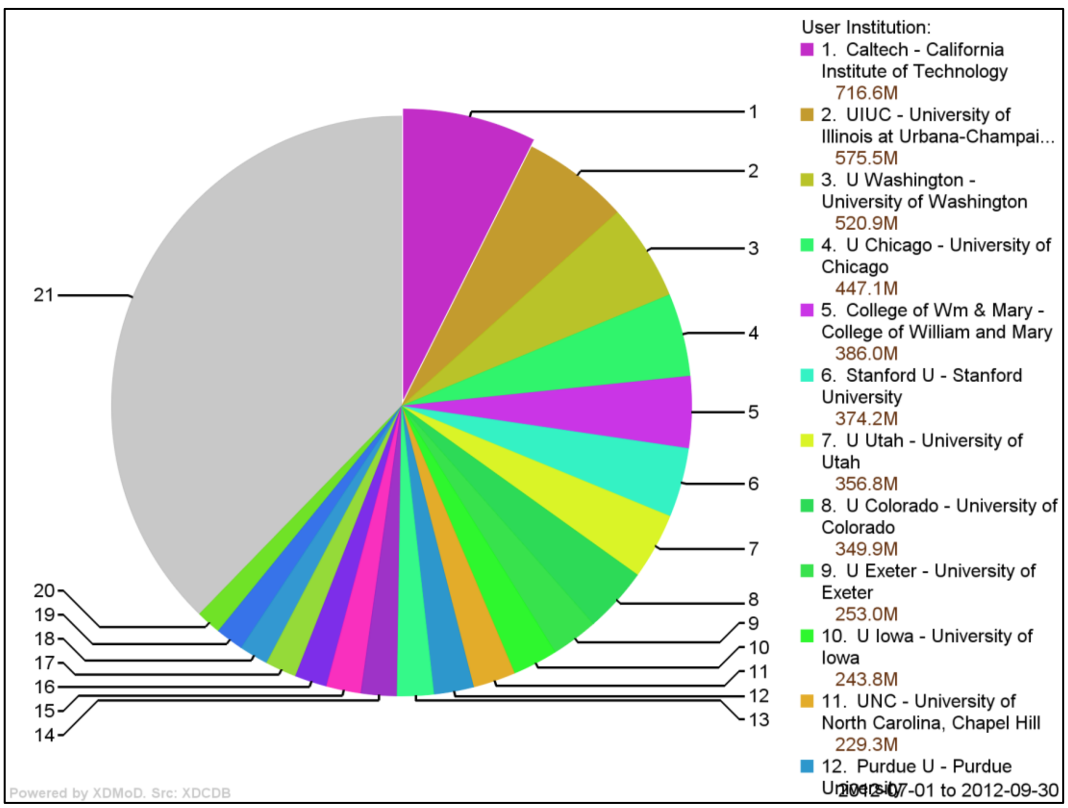


Figure 24: Resource consumption in mega-normalized units ($1e^6$) by institution in mega-normalized units for Kraken in Q2PY2.

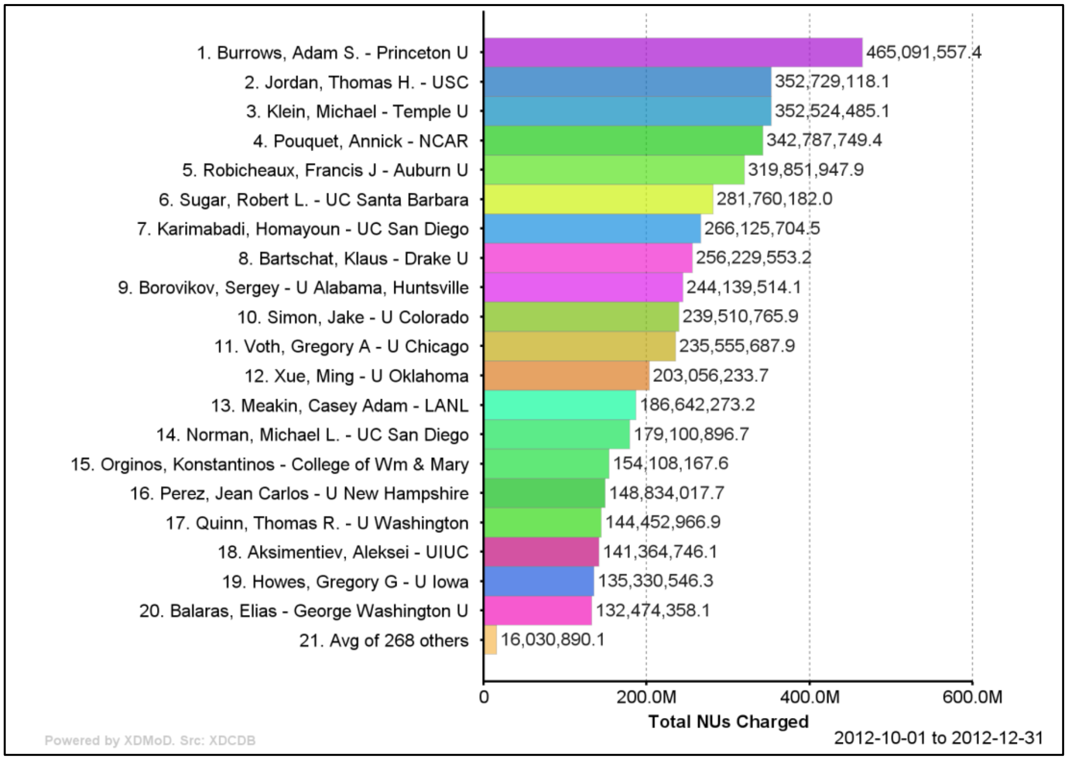


Figure 25: Resource consumption by PI in Mega-normalized units for Kraken in Q2PY2.

16.9.2.1 Nautilus

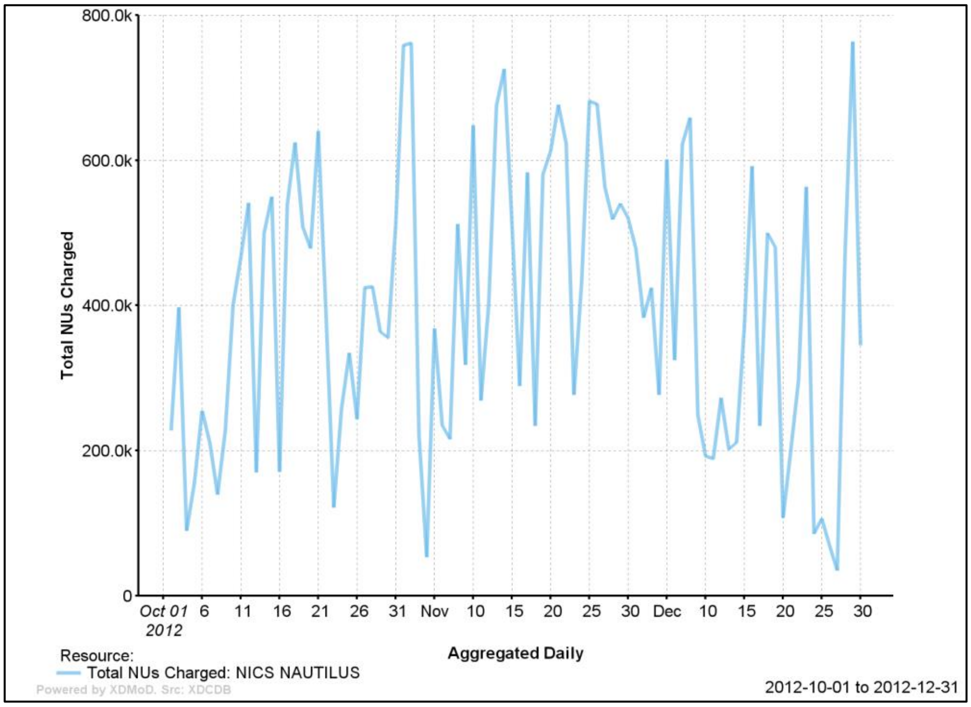


Figure 26: Daily resource consumption in kilo-normalized units ($1e^3$) charged on Nautilus in Q2PY2.

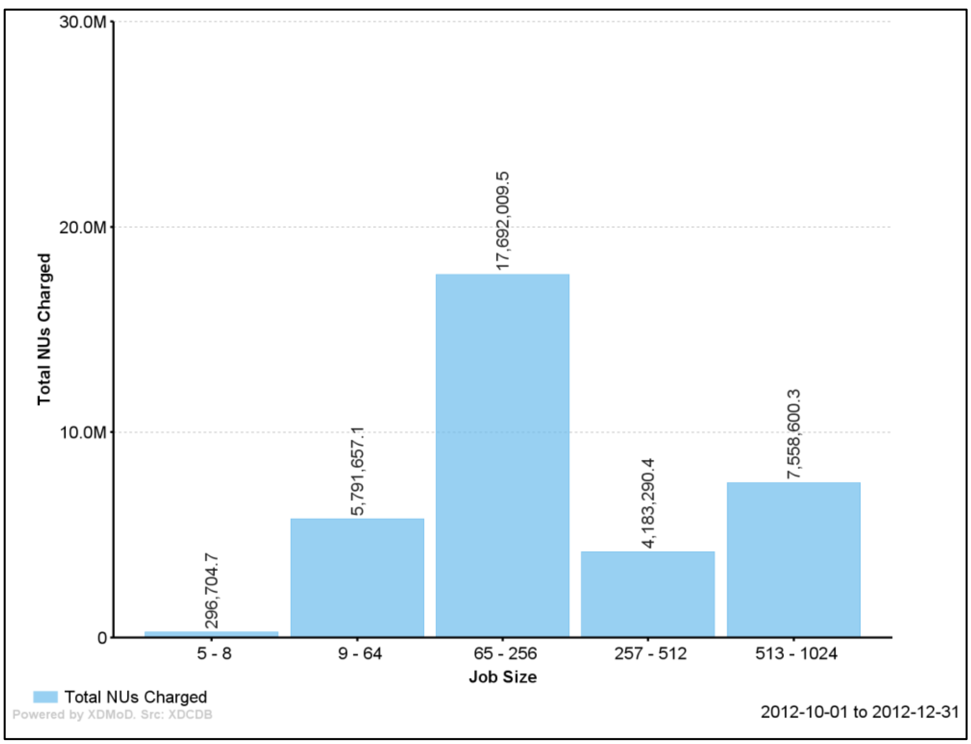


Figure 27: Total resource consumption in mega-normalized units ($1e^6$) by job size for Nautilus in Q2PY2.

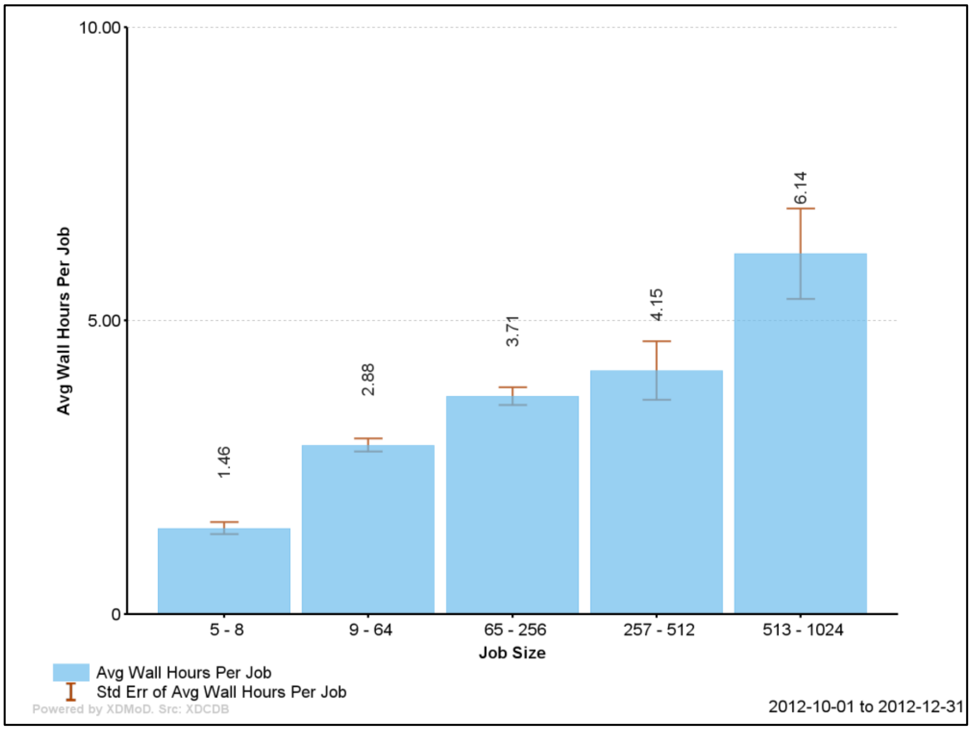


Figure 28: Average wall time in hours by job size on Nautilus in Q2PY2.

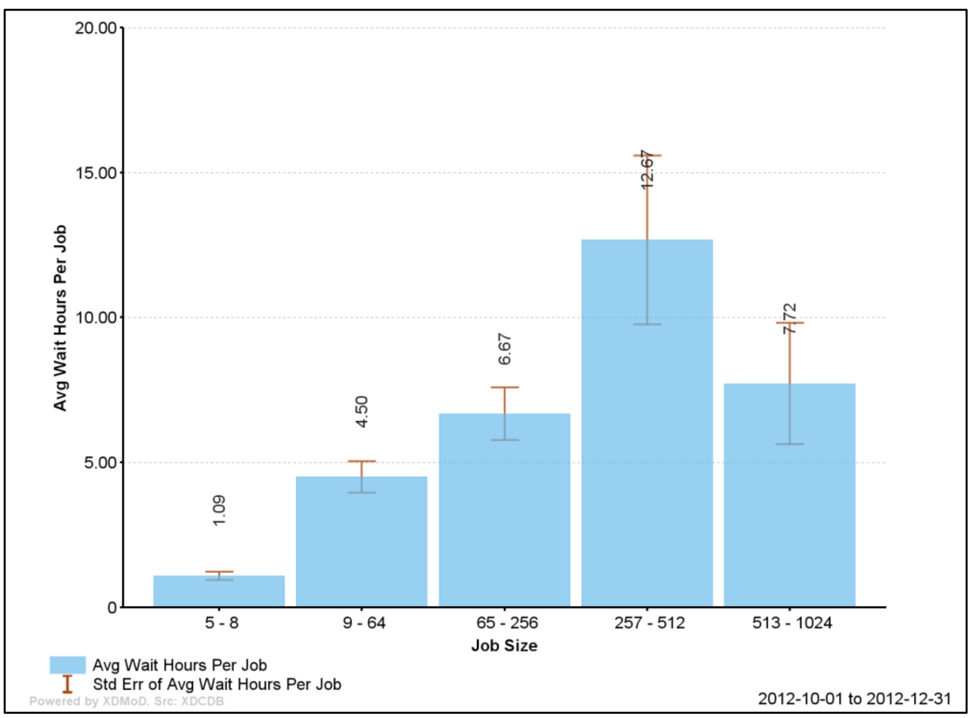


Figure 29: Average wait time in hours by job size for Nautilus in Q2PY2.

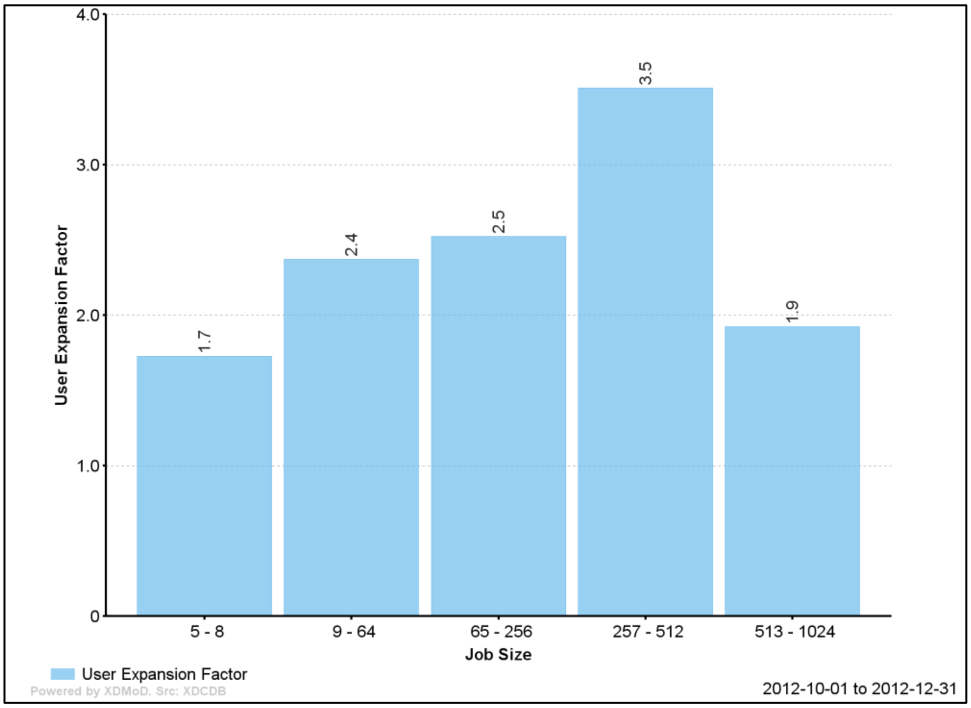


Figure 30: Expansion factor by job size for Nautilus in Q2PY2.

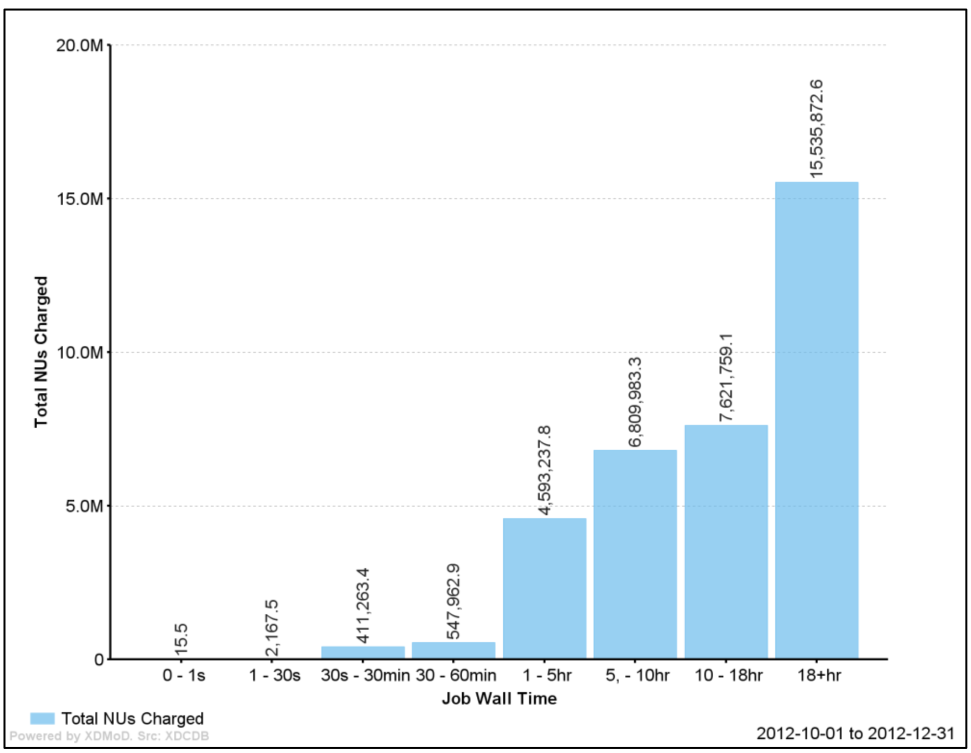


Figure 31: Total resource consumption in mega-normalized units (1e6) by wall time for Nautilus in Q2PY2.

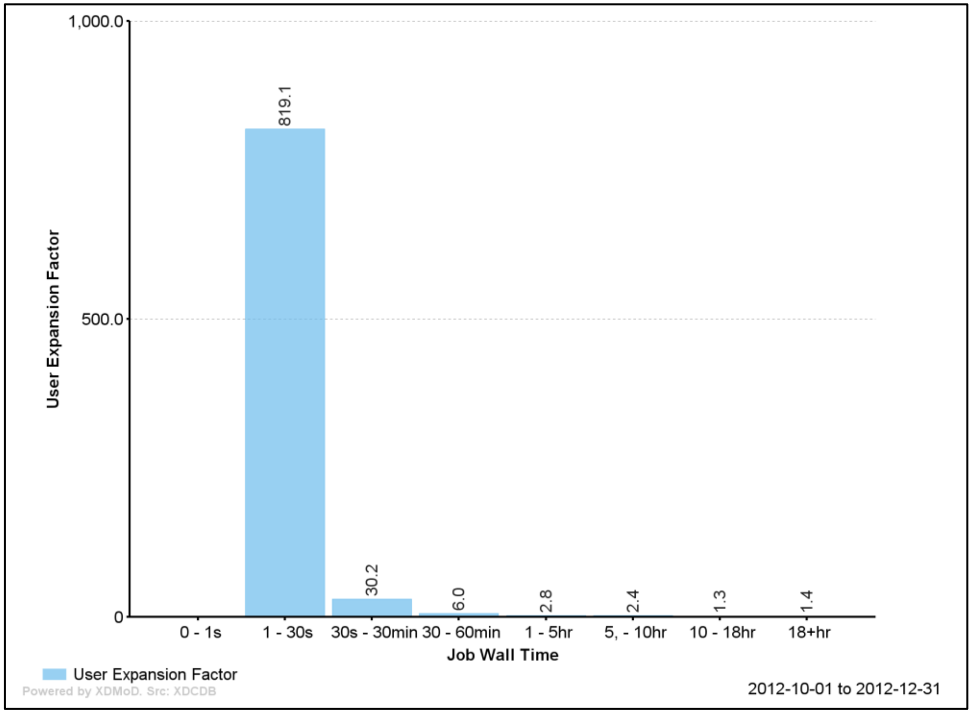


Figure 32: Expansion factor by wall time for Nautilus in Q2PY2.

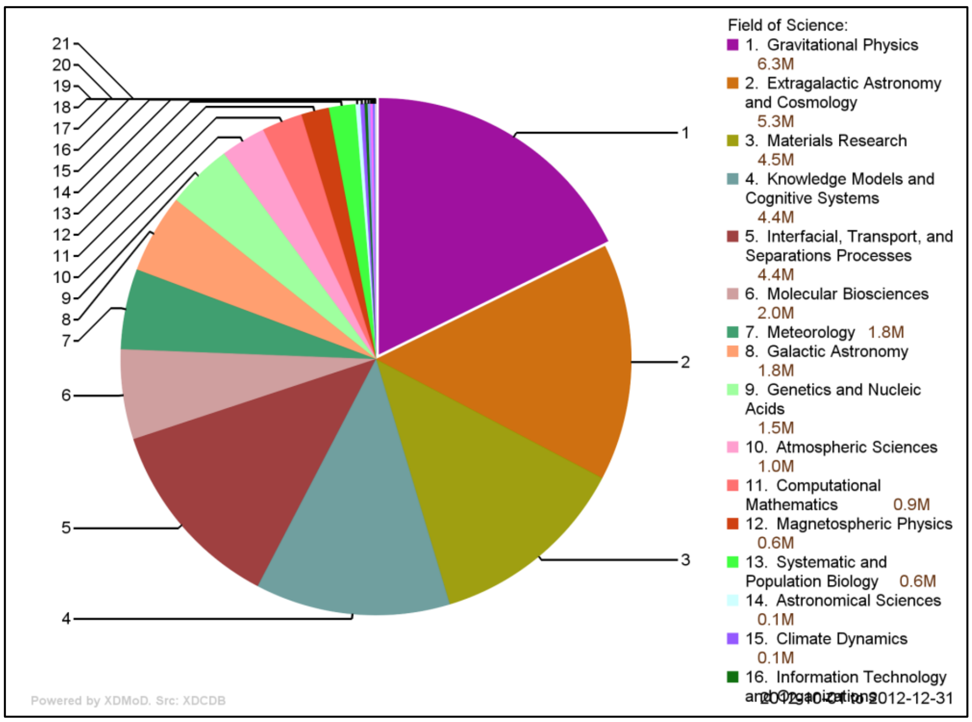


Figure 33: Resource consumption by scientific domain in mega-normalized units for Nautilus in Q2PY2.

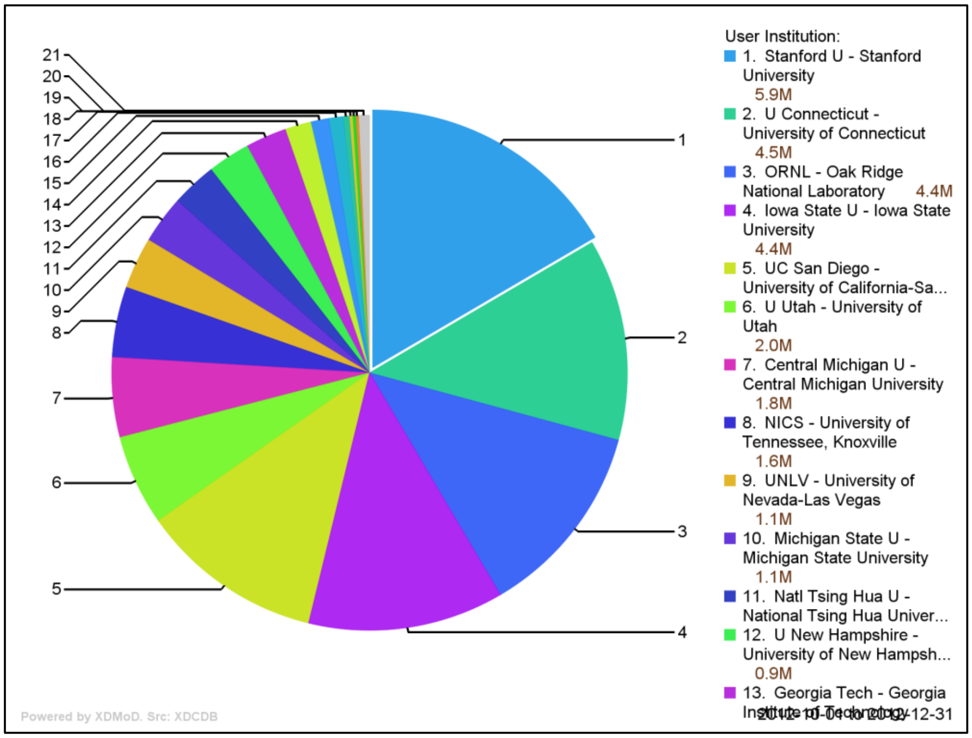


Figure 34: Resource consumption by institute in mega-normalized units for Nautilus in Q2PY2.

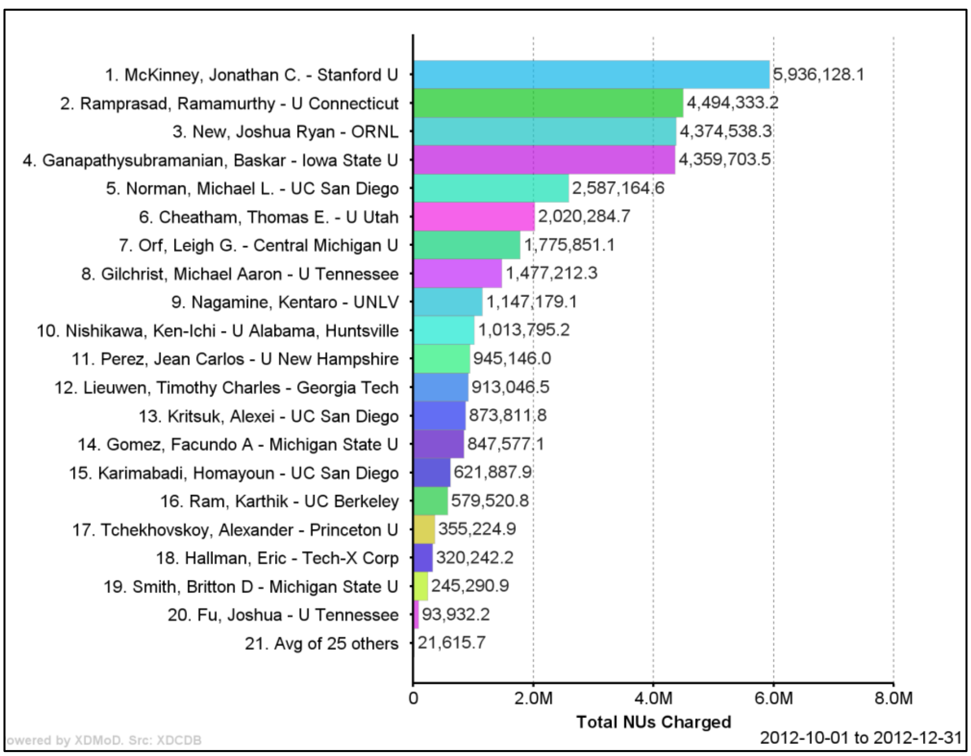


Figure 35: Resource consumption by PI in mega-normalized units for Nautilus in Q2PY2.

16.9.3 *Standard User Assistance Metrics*

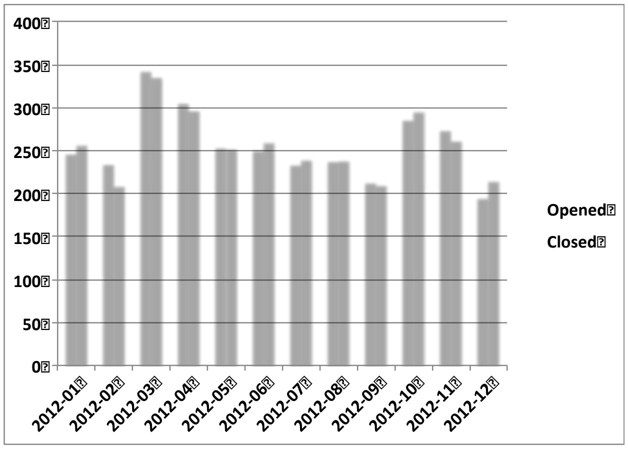


Figure 36: XSEDE tickets opened/closed by month.

NICS' front line user support responded to 758 new XSEDE tickets in the quarter (

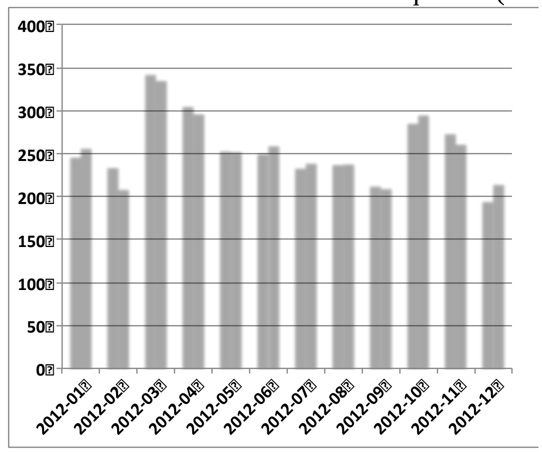


Figure 36) and closed 776 tickets. These tickets corresponded to a variety of issues (Table 14) with the majority falling into two groups: login/access issues and jobs/batch queues. Open tickets experienced a MTTR of 32.3 hours for the quarter.

Table 14: Ticket resolution times by category for Q2PY2.

Category	Oct-12	Nov-12	Dec-12	Total
Login / Access Issues	125	87	79	**291**
Jobs / Batch Queues	56	77	48	**181**
Software	38	32	24	**94**
Archival Storage Issues	11	9	6	**26**
File Systems	10	19	13	**42**
Account Issues	27	17	11	**55**
System Issues	7	13	6	**26**
Other	9	15	9	**33**
Grid Software	1	4		**5**
Network Issues	1	1		**2**
INCA Messages	1		1	**2**
Community Software Area Requests				**0**
Reservation Request		1		**1**
Total	**286**	**275**	**197**	**758**

16.9.4 *SP-specific Metrics*

NICS' resources provided roughly 55% of computational cycles that were delivered to the NSF community in this quarter (Figure 38), and NSF charges accounts for most of the total charges on these resources (Figure 37 and Figure 38).

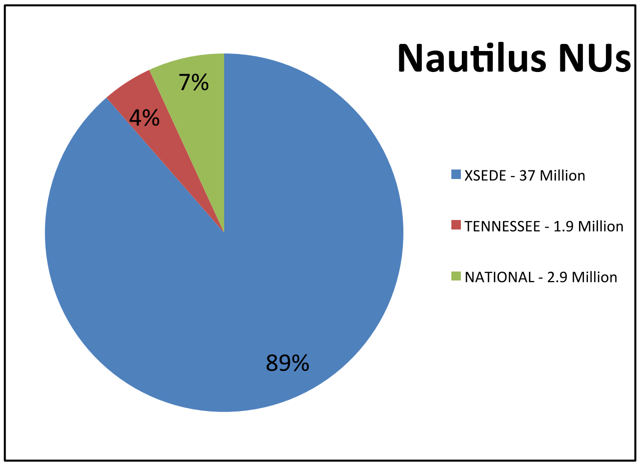


Figure 37: XSEDE charges as a percentage of total charges on Nautilus in Q2PY2.

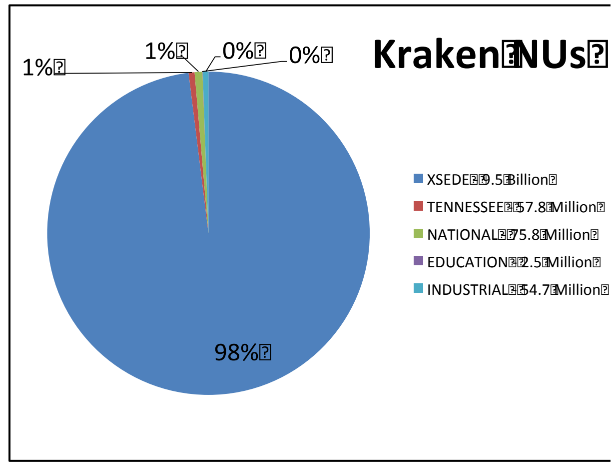


Figure 38: XSEDE charges as a percentage of total charges on Kraken in Q2PY2.

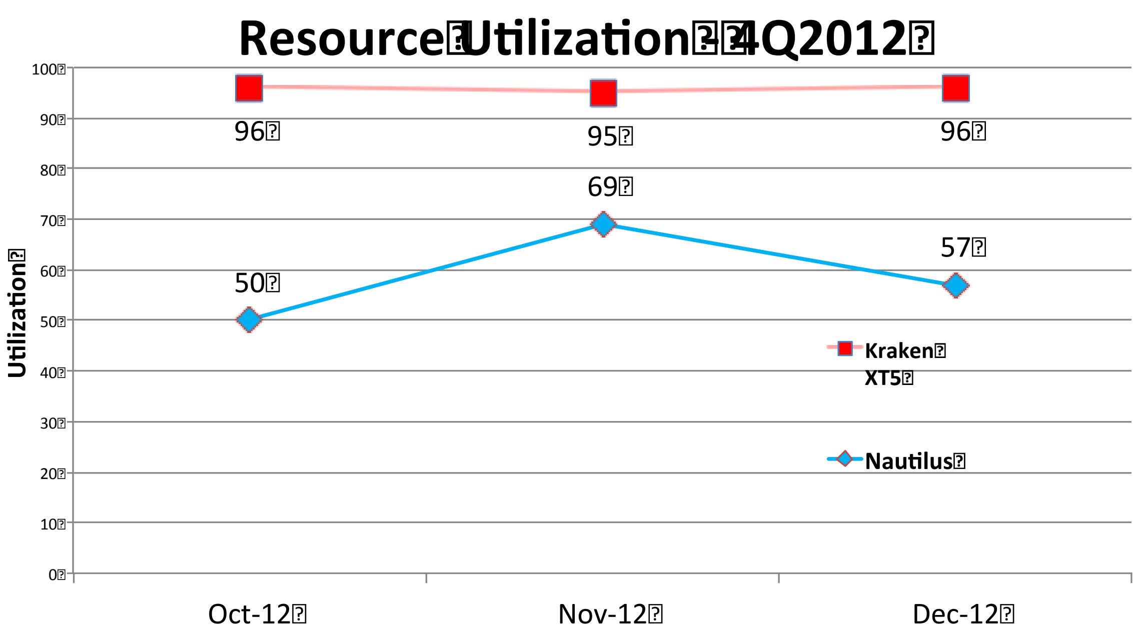


Figure 39: Monthly utilization for Kraken and Nautilus in Q2PY2.

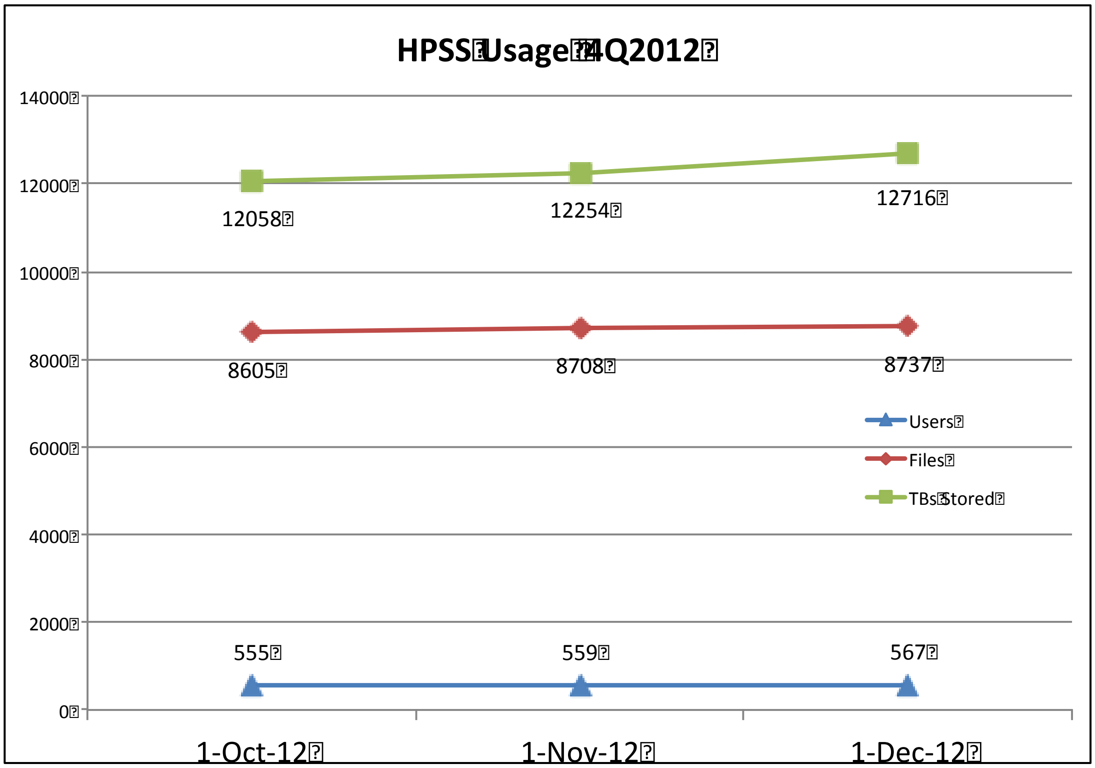


Figure 40: Archival storage usage on HPSS for Q2PY2.

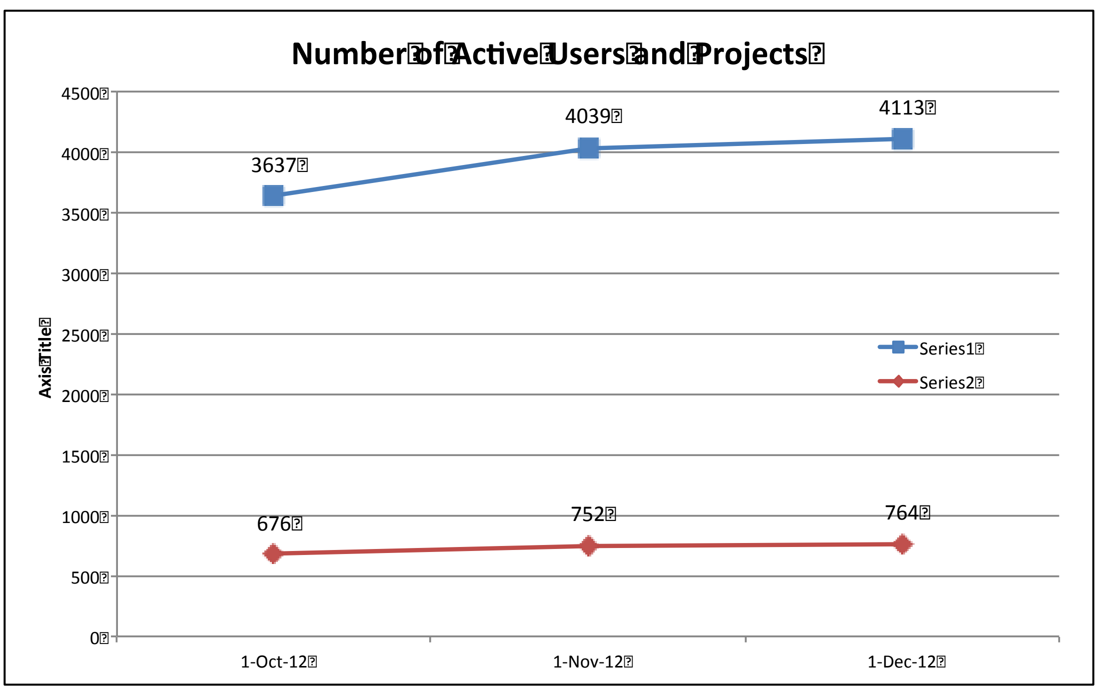


Figure 41: Number of active users and projects on NICS resources at the end of Q2PY2.

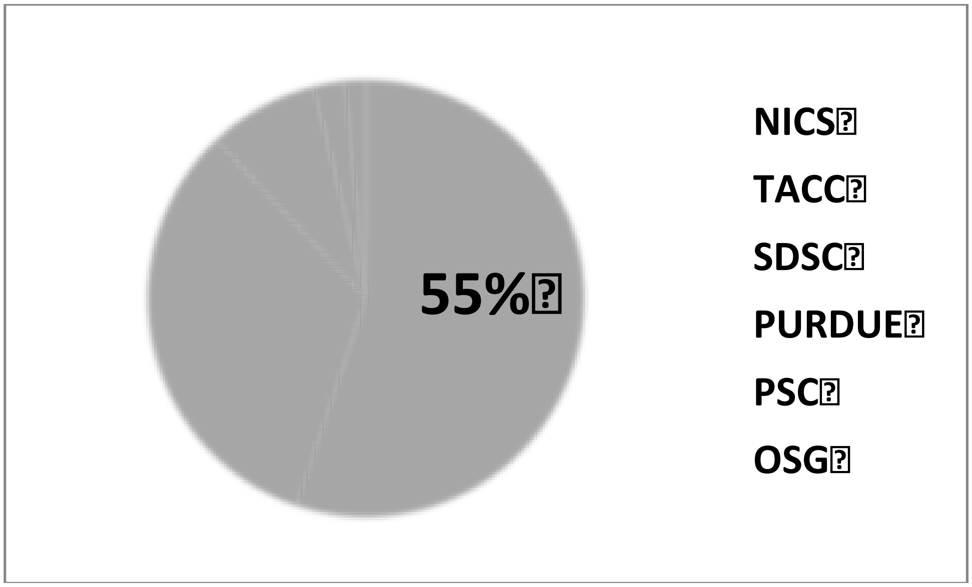


Figure 42: CPU hours delivered by NICS resources as a percentage of total CPU hours delivered by XSEDE resource in Q2PY2.

17 Pittsburgh Supercomputing Center - Service Provider Quarterly Report

17.1 Executive Summary

The Pittsburgh Supercomputing Center (PSC) installed *Sherlock*, a YarcData uRiKA™ (Universal RDF Integration Knowledge Appliance) data appliance with PSC enhancements. An experimental system funded via NSF's Strategic Technologies for Cyberinfrastructure program, *Sherlock* enables large-scale, rapid graph analytics as well as support for heterogeneous applications. *Sherlock* contains 32 YarcData Graph Analytics Platform nodes, each containing 2 Threadstorm 4.0 processors, a SeaStar 2 interconnect ASIC, and 32 GB of RAM plus additional Cray XT5 nodes having standard x86 processors. PSC operates and supports *Blacklight*, a powerful and unique resource for the national research community. *Blacklight*, an SGI Altix UV 1000 acquired with the assistance of an NSF grant and operated as an XSEDE resource, is the world's largest shared-memory system, providing two partitions of 16TB each. With operational funding from NIH, PSC also operates *Anton*, a special-purpose computer for molecular dynamics which is used by many NSF-supported researchers. PSC systems are supported by a central file system *Brashear* (except for Sherlock), and extensive LAN, MAN and WAN infrastructure. For persistent storage such as archiving files, hosting data collections, etc., PSC operates Data Supercell, a scalable, disk-only file repository that provides fast access to files. Its initial deployment has four petabytes.

PSC resources enabled significant progress in many areas; e.g., genomics, biochemistry and chemistry. Users are finding *Blacklight's* operating characteristics to be very valuable. For instance, Mostafa Elshahed (Oklahoma State University) had a job that used 7,167 GB, a record, and jobs that use more than 2 terabytes are common.

PSC people make significant intellectual contributions and continue to earn high praise for their efforts. For example:

- Jeff Pummill (University of Arkansas) commented, "PSC is far and away the most responsive to users from what I can tell."
- Mike Widom (CMU) said, "PSC has been an invaluable asset to my research … I have benefited from a long-standing association with PSC staff member Yang Wang that has resulted in joint publications and joint research support …"
- The patent application of PSC staff members for the Zest parallel storage system issued as a United States Patent on November 20, 2012.

Although users gave many compliments to PSC in the 2012 XSEDE User Satisfaction Survey, they also pointed out areas for improvement. In response, PSC is re-orienting its user documentation toward less experienced HPC users as well as the more experienced ones, and providing more information on job scheduling practices and machine status.

PSC engaged in a range of Training, Education and Outreach activities, which included enlisting new communities into HPC, major STEM education programs including outreach to under-represented communities, and HPC training workshops. Specifically, PSC has assumed leadership in training on programming and support for accelerators.

17.1.1 *Resource Description*

Computing and Storage: PSC provides a range of computing and storage platforms for the national science community.

PSC acquired and installed *Sherlock*, a YarcData uRiKA™ (Universal RDF Integration Knowledge Appliance) data appliance with PSC enhancements. It is an experimental system funded via NSF's Strategic Technologies for Cyberinfrastructure (STCI) program. *Sherlock* enables large-scale, rapid graph analytics through massive multithreading, a shared address space, sophisticated memory optimizations, a productive user environment, and support for heterogeneous applications. *Sherlock* contains 32 YarcData Graph Analytics Platform nodes, each containing 2 Threadstorm 4.0 (TS4) processors, a SeaStar 2 (SS2) interconnect ASIC, and 32 GB of RAM. Aggregate shared memory is 1 TB, which can accommodate a graph of approximately 10 billion edges. The TS4 processors and SS2 interconnect contain complementary hardware advances specifically for working with graph data. These include support for 128 hardware threads per processor (to mask latency), extended memory semantics, a system-wide shared address space, and sophisticated optimizations to prevent "hotspots" involving contention for data. PSC has customized *Sherlock* with additional Cray XT5 nodes having standard x86 processors to add valuable support for heterogeneous applications that use the Threadstorm nodes as graph accelerators. This heterogeneous capability will enable an even broader class of applications, including genomics, astrophysics, and structural analyses of complex networks. Other x86 nodes serve login, filesystem, database, and system management functions. There are two main ways of using *Sherlock*: using the uRiKA™ data appliance for performing complex graph analytics, or running other applications that benefit from the Graph Analytics Platform architecture.

For applications requiring very large shared memory, high-productivity programming models, and/or moderate parallelism with a high-performance system-wide interconnect, PSC operates *Blacklight*, an SGI UV 1000 cc-NUMA shared-memory system comprising 256 blades. Each blade shares 128GB of local memory, and holds two Intel Xeon X7560 (Nehalem) eight-core processors, for a total of 4,096 cores and 32 TB across the whole system. Each core has a clock rate of 2.27 GHz, supports two hardware threads and can perform 9 Gflop/s for a total system floating point capability of 37 Tflop/s. *Up to 16 TB of this memory is accessible as a single memory space to a shared-memory program.* Message-passing and PGAS programs can access all 32 TB on the system. *Blacklight* is part of the National Science Foundation XSEDE integrated national system of cyberinfrastructure.

Additionally, PSC has an SGI Altix 4700 system called *Salk*, smaller than *Blacklight*, which is also targeted at applications requiring large shared memory, high-productivity programming models, or moderate parallelism with a high-performance, system-wide interconnect. *Salk* is administered for the NIH-funded National Resource for Biomedical Supercomputing (NRBSC) and offers 144 Montvale processors providing a peak aggregate speed of 0.96 Tflop/s with 288 GB shared memory. This system supports advanced programming languages and models including UPC and Star-P.

PSC operates an *Anton* special-purpose supercomputer for molecular dynamics (MD) simulation that performs up to 100 times faster than conventional supercomputers. Designed by D. E. Shaw Research (DESRES) and provided to PSC without cost by DESRES, it is available for non-commercial research use by universities and other non-profit institutions. This machine, the only *Anton* computer operated outside DESRES, is hosted by PSC and is available to the national biomedical community with funding from NIH's National Institute of General Medical Sciences. Computing time on *Anton* is allocated by a peer-review committee convened by the National Research Council. A large number of *Anton* users are NSF-supported investigators. The *Anton* computer is supplemented by a high performance file storage system for simulation trajectories and an analysis cluster (*Kollman*). Each of the four nodes in the analysis cluster consists of two Intel Westmere six-core processors and 96 GB of memory. The high-performance file storage system consists of a 500-TB Lustre file system. The file system and the analysis cluster nodes are interconnected over Quad Data Rate (QDR) InfiniBand. Availability of the *Anton* system has been extended until September 2014.

PSC operates several Linux clusters for scientific research as well as several high-end servers and powerful workstations for development, analysis, and visualization tasks.

The production workload on all of the PSC computing platforms is managed by PBS/Torque. Several scheduler policy modules used include a locally-developed module, *Simon*, and the Maui scheduler.

All of the PSC computing platforms except *Sherlock* have access to *Brashear*, PSC's shared, central file system using the Lustre file system architecture. It comprises eight storage nodes and 350 TB of direct-attached disks, forming a large I/O cluster globally accessible within the PSC site. Access to the file system is provided by InfiniBand, 10-Gigabit Ethernet and 1-Gigabit Ethernet. Each node in the I/O cluster is a Lustre Object Storage Server (OSS) hosting multiple Object Storage Targets (OSTs).

PSC had been a partner in the Lustre *Albedo* Wide Area File System project that was decommissioned during the report period. PSC took the lead by managing the metadata service for *Albedo* in addition to providing a portion of its bulk object storage.

PSC's Data Supercell for persistent storage of information is a disk-only file repository that is less costly than a disk-tape archive system and provides much faster file access. Each building block in the repository has one petabyte of useable disk storage, which is managed by the ZFS file system and the PSC-developed SLASH2 replicating distributed file system. ZFS and SLASH2 provide multiple layers of robust data integrity checking to protect user data against data corruption. This building-block architecture will enable the repository to scale well beyond its initial deployment of four petabytes.

Users can access the repository from within PSC using the familiar PSC file archiving utility, *far*. From outside PSC, users can employ a variety of well-known file transfer methods such as SCP and GridFTP. These transfers are handled by a series of dedicated data transfer servers.

Networking: PSC network facilities consist of production and research Local Area Network (LAN), Metropolitan Area Network (MAN), and Wide Area Network (WAN) infrastructures.

> *Local Area Network Infrastructure* - The LAN infrastructure consists of switched Ethernet with speeds up to 10 Gb/s. The LAN architecture was constructed to overcome issues of buffer contention in data center Ethernet switches on the Science DMZ[1]. This allows for higher bandwidth data transfers to the data transfer nodes.

3 Rivers Optical Exchange: PSC operates and manages the 3 Rivers Optical Exchange (3ROX) a regional network aggregation point that provides high-speed commodity and research network access, primarily to sites in Western and Central Pennsylvania and West Virginia. While the primary focus of 3ROX is to provide cost-effective, high-capacity, state-of-the-art network connectivity to the university community, this infrastructure also provides well-defined network services to both community (K-12, government) and commercial entities in Western Pennsylvania. University member sites currently include Carnegie Mellon University, the Pennsylvania State University, the Pittsburgh Supercomputing Center, the University of Pittsburgh, WVnet, and West Virginia University.

> *3ROX Metropolitan Area Network Infrastructure* - 3ROX MAN infrastructure is DWDM-based and supports multiple 10-Gigabit Ethernet waves. It is capable of supporting 40- and 100-Gigabit waves as the need arises. This DWDM network connects four different locations

[1] From http://fasterdata.es.net/science-dmz/: The Science DMZ is a portion of the network, built at or near the campus or laboratory's local network perimeter that is designed such that the equipment, configuration, and security policies are optimized for high-performance scientific applications rather than for general-purpose business systems or "enterprise" computing.

around the city that include long haul service providers, a co-location hotel, a campus based co-location facility, and the Northern Pike machine room.

3ROX Wide Area Network Infrastructure - 3ROX WAN infrastructure has both Commodity Internet and Research and Education components. Explicit routing is used to maintain the acceptable use policies associated with the various production and research network infrastructures.

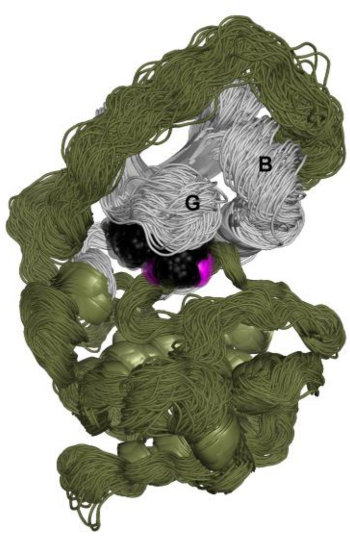
The 3ROX Commodity Internet component consists of multiple high-performance WAN connections to major Internet service providers, including a Gigabit Ethernet connection to Cogent and a 10-Gigabit Ethernet connection to Level 3. In addition, 3ROX provides connectivity to both regional and national Internet2 and content peering infrastructures, in particular access to the Internet2 based TR/CPS content peering services; regional peering with Southern Cross Roads (SOX), OARnet and Comcast; along with a recent direct peering connection with Google.

The 3ROX Research and Education component includes a 10-Gigabit Ethernet connection, with 5 Gb/s of bandwidth, to the Internet2 network. In addition to the Internet2 connection, 3ROX also has a 10-Gigabit Ethernet connection to National LambdaRail; a 10-Gigabit Ethernet connection to the XSEDE backbone network; a 10-Gigabit Ethernet connection between PSC's offices and its remote supercomputing machine room at 4350 Northern Pike; and a 10-Gigabit Ethernet connection to Penn State University (PSU) to provide XSEDE connectivity to PSU.

17.2 Science Highlights

In addition to major science accomplishments that are highlighted in the XSEDE report, we present selected others specific to PSC.

17.2.1 <u>Biochemistry and Molecular Structure and Function: Mapping Slow Dynamical Regulation of a Protein Kinase by Combining Molecular Dynamics with NMR Data (Susan Taylor & Chris Taylor, University of California, San Diego)</u>



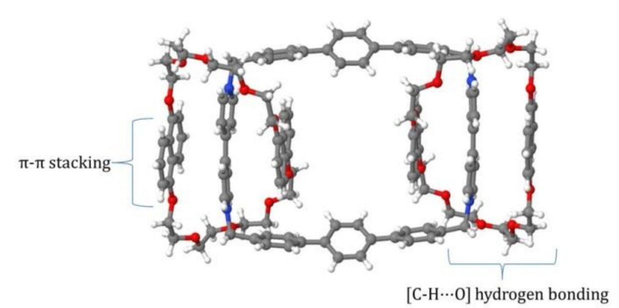
This graphic shows overlaid snapshots from one of the simulations. The two main structural components of PKA's catalytic domain, the N-lobe (light gray) and C-lobe (dark green), enclose the "active site," which holds ATP (black) and two magnesium ions (purple). The image, observes McClendon, shows that PKA's glycine-rich loop (G) and nearby B-helix (B) "aren't locked down by the ATP and two magnesiums, but instead remain more flexible than we expected."

Protein kinase A (PKA) is one among a superfamily of enzymes, the kinases, which play a central role in regulating the complex network of chemical reactions within the cell. The kinases are ubiquitous in living things. "Protein kinases operate like stop and go signals," says Susan Taylor, professor of chemistry and biochemistry at the University of California, San Diego. "They are essential molecular switches for all biology." PKA is the prototype of this big family, a protein for which Taylor and her colleagues first solved the structure in 1991. With this structure as a map, Taylor's research group has answered many questions about how protein kinases regulate cell metabolism by means of phosphorylation. By phosphorylating a variety of target proteins, PKA helps regulate memory, cell growth and many other processes.

When kinases go awry, diseases are often the result — especially cancer. For this reason, the kinase superfamily, with PKA as prototype, is a prominent target for drug therapy, and several effective anti-cancer drugs that work by blocking the active site of defective kinases are already available. To advance this work, Taylor and post-doctoral researcher Chris McClendon used *Anton* to simulate several different states of PKA's catalytic domain, which binds with ATP and releases ADP. NMR studies by Gianluigi Veglia at the University of Minnesota, in collaboration with the Taylor lab, showed that these processes occur on slow biological timescales of milliseconds. With availability of *Anton*, McClendon was, for the first time, able to glean useful information from MD simulations about these cyclical structural changes. A key finding was that the tail of the C-lobe, at the top of the PKA structure, flips open and closed like a latch to hold and release a "gylcine-rich loop" that closes over the ATP. The simulations also suggest that active-site opening and closing can occur at rates faster than expected from prior studies. "We're getting new clues as to what regions are dynamic," says Taylor. "It's the first time we can do calculations at a timescale we can experimentally validate. *Anton* provides us with a way to test the consequences of disease mutations and engineered mutations on the overall dynamics, which we have never been able to do."

17.2.2 Chemistry: The Nature of Noncovalent Interactions in Catenane Supramolecular Complexes: Calibrating the MM3 Force Field with ab initio, DFT and SAPT Methods (Tomekia Simeon, Department of Chemistry, Northwestern University)

Various types of noncovalent interactions are responsible for the assembled architecture of interlocked molecules such as catenanes and rotaxanes. Important noncovalent interactions in these supramolecular complexes are the [C-H···O] hydrogen-bonding and the π-π stacking interactions. With the goal of determining if molecular mechanics (MM3) can provide accurate estimates of these interactions, Tomekia Simeon's team examine [3] catenane[1] **2**·$4PF_6$ using MM3, *ab initio* methods (HF, MP2), several versions of density functional theory (DFT), and symmetry-adapted perturbation theory (SAPT). The methodology can then be extended to larger catenane and rotaxane structures. They first consider MP2 and DFT methods to determine the strengths of [C-H···O] hydrogen-bonding and π-π stacking interactions, including a systematic study of the effect of density functional and basis sets on the interactions. They then use these results to calibrate the MM3 force field. These comparisons show that the MM3-calculated complexation energies agree qualitatively with the QM energetic ordering, with quantitative differences that are comparable to differences obtained between results of nominally comparable density functionals. *The MM3 results are in excellent agreement with those from DFT-SAPT for both interactions*, closer than with the DFT results, showing that the DFT functionals still need improvement for these interactions. They use DFT-SAPT to decompose the interaction energies into components. *They find that the electrostatic interactions dominate the [C-H···O] hydrogen-bonding interactions, while dispersion makes a significant contribution to π-π stacking*. In addition, both of these interactions are enhanced by the charged bipyridinium, compared to what would be obtained for an uncharged structure. The simulations required large memory capabilities. Using the software *Molpro*, the runs used approximately 99.9% of the 256 GB available on 32 cores on *Blacklight*.



The crystallographic structure of [3] catenane, illustrating regions of π-π stacking and [C-H···O] hydrogen-bonding interactions. The color labels for the atoms are carbon (gray), oxygen (red), nitrogen (blue) and hydrogen (white).

Simeon says, “We are extremely grateful to the PSC staff for their support with running *Molpro* successfully on *Blacklight*.”

Reference

1. Houk, K. N.; Menzer, S.; Newton, S. P.; Raymo, F. M.; Stoddart, J. F.; Williams, D. J. *J. Am. Chem. Soc.* **1999**, *121*, 1479-1487.

17.3 User-facing Activities

17.3.1 System Activities

Sherlock: *Sherlock*, a YarcData uRiKA™ data appliance with PSC enhancements is an experimental system funded via NSF’s Strategic Technologies for Cyberinfrastructure (STCI) program. Sherlock arrived at PSC on November 27 and was installed on November 29. We began immediately working with some of the early users who contributed to our STCI proposal. Others were notified, and still others are turning up rapidly through discussions. YarcData experts Steve Reinhardt and Jim Maltby came to PSC on December 3-5 to provide training on uRiKA and (for Graph Analytic Platform nodes) C++ training to PSC staff and local users.

Large Memory Usage on *Blacklight*: Users continue to take advantage of the large shared memory on *Blacklight*. In early November Mostafa Elshahed of Oklahoma State University (genomics) had a job on *Blacklight* that used 7,167 GB, a record, and ran for 138.24 hours. In most weeks there are several jobs that use more than 1 TB, and jobs that use more than 2 TB are common. For instance, in the reporting period Renyue Cen of Princeton University (cosmology) had many jobs over 2 TB, one using 3,490 GB and running for 128.79 hours. Also, regarding his team’s parallelized FFT code for solving full field stress-strain problems in materials, Tony Rollett, CMU Materials Science & Engineering, said, “Access to a large shared memory machine was and is particularly useful.”

17.3.2 Services Activities

Appreciation of PSC: PSC continues to receive comments on the helpfulness of PSC staff members and the intellectual contributions that PSC brings to users. The paragraphs below are comments that we received in this reporting period.

Jeff Pummill, University of Arkansas High Performaqnce Computing Center: Last quarter, PSC reported on the work by Jeff Pummill, et al of the University of Arkansas on whole genome sequencing of the Timber Rattlesnake. In a subsequent email, Pummill commented, “PSC is far and away the most responsive to users from what I can tell.” He specifically mentioned that what makes *Blacklight* especially useful “is the ability to run longer jobs (and to have a few hours added to the runtime if necessary...).”

Gordon Rule, CMU Biological Sciences: Shantanu S. Bhattacharyya of Gordon Rule’s group in the Department of Biological Sciences at Carnegie Mellon University wrote to PSC’s Marcela Madrid with respect to running CHARMM on *Blacklight*, “The code worked perfectly. I simply cannot thank you enough for your help. Thanks a lot again for your help with my simulations.”

Mike Widom, CMU Physics, Materials Science & Engineering: “The PSC has been an invaluable asset to my research in computational Condensed Matter Physics. In recent years I benefited greatly from the abilities of an undergraduate researcher, Max Hutchinson, who had previously gained experience in supercomputing while working at the PSC. Max built on this experience to devise a memory efficient algorithm for counting rhombus tilings of an octagon. This was then run on *Blacklight* at the PSC utilizing the large shared memory capability to reach previously unattainable sizes. In a separate project, the same undergraduate used his GPU programming experience, also gained at the PSC to port the first-principles code VASP to run on GPU systems.

We benchmarked performance of a GPU system against multi-core runs on *Blacklight* to demonstrate the capability of the GPU. This GPU project resulted in a publication and also a small research grant. Finally, I have benefited from a long-standing association with PSC staff member Yang Wang that has resulted in joint publications and joint research support for a variety of projects utilizing first principles computational techniques including most recently investigation of high entropy alloys."

Tatyana Mamonova, Pitt School of Medicine: "We used the PSC resources to run Amber simulations on NHERF1 (the scaffolding protein Na+/H+ Exchange Regulatory Factor-1) PDZ1/PDZ2-ligand systems, and the help of Marcela Madrid with the software (pmemd.MPI, TI) was very valuable in getting the simulations running on nanosecond time scale (*Pople* and *Blacklight*). We successfully modeled the NHERF1 PDZ1/PDZ2 domains in the bound state with the carboxy-terminal, five-amino acid residue peptides of its potential targets, including parathyroid hormone receptor (PTHR) and the type II sodium-dependent phosphate co-transporters (Npt2a) (Biochemistry, 51, 3110-3120, 2012). MD simulation results are in good agreement with experiment. Our findings offer new insights into intermolecular interaction and intracellular trafficking of NHERF1 (J. Biol. Chem., 287, 24148-24163, 2012)."

Tony Rollett, CMU Materials Science & Engineering: "PSC has been crucial to our development of the parallelized FFT code for solving full field stress-strain problems in materials. This code is proving essential to solving problems in tin whisker growth, thermal stresses in thermal barrier coatings, plasticity and damage accumulation in Zr, Cu, sheet steel and fatigue crack initiation in superalloys. Access to a large shared memory machine was and is particularly useful. Expert help from PSC staff also contributed significantly."

Catalina Achim, CMU Chemistry: "Our collaboration with PSC was very beneficial not only for the research itself but also for educational purposes. Working with Marcela Madrid, my graduate students learned how to do molecular dynamics simulations. We are always anxious to get results and push the limits of our knowledge. Access to PSC computer resources and, even more, the help of Marcela made a huge difference in how fast we got the answers we were seeking."

Prahlad Menon-Gopalakrishna, Grad Student of Kerem Pekkan, CMU Biomedical Engineering: "The documentation has been helpful. I also actively interact with David O'Neal who has mentored me regarding appropriate use of the PSC resources and has been a great support through the past year."

Hy Trac, CMU Physics: "Thank you for all the help with *Blacklight* over the past year… This collaboration between CMU and the PSC has culminated in 3 papers (part of a series of at least 5 papers) that just showed up together on the astro paper archive. Multiple submissions like this are rare even for large collaborations with > 50 people, so being able to do it with our small team is a proud accomplishment. We thank you and the PSC in the Acknowledgements."

Documentation and Status Information: Last quarter, PSC reported that in response to the 2012 XSEDE User Satisfaction Survey, we are reviewing our practices and procedures in the following areas:

- Re-orient PSC user documentation to account for less experienced HPC users as well as the more experienced ones.
- Provide more information to users on *Blacklight's* operational status and make it readily accessible.
- Provide more specific information on our job scheduling practices.
- Provide tools for users to get more information on the scheduling status of their jobs.

These are the steps PSC has taken so far:

- Working on an "Introduction to Supercomputing for Novices" document.
- Working on a document and FAQ giving an overview of our genomics packages.
- Now providing a weekly status report on Tuesdays concerning important system events planned for the following week and reporting other relevant information concerning PSC practices and procedures. Report goes to XSEDE News and to PSC's social media outlets Facebook, Twitter, and the PSC blog.
- Added information about commands for job status and system monitoring to the *Blacklight* user document. Further work to improve this documentation is underway.
- Added information about limits on 16-core jobs to the *Blacklight* user document.
- Implemented improvements to the clarity and informativeness of our job and system status commands. We are working on further improvements.
- Significantly expanded and improved the XSEDE User Guide on Data Supercell by making it identical to PSC's local documentation. Over time we will make all PSC-related XSEDE documentation identical to our local documentation.
- Improved our parallel debugger (idb) documentation. A request was posted to the email list of *Blacklight* users, asking if they need Totalview or DDT debuggers in addition to idb.
- Talked to Warren Smith (TACC) about feeding *Blacklight's* job status information to the *Karnak* queue prediction engine, which feeds a display in the XSEDE User Portal of queue predictions for queued jobs. Smith is working on a new version of *Karnak* and will let PSC know when he's ready to test the feed from *Blacklight*.

17.4 Security

PSC had no security incidents.

17.5 Education, Outreach, and Training Activities

Type	Title	Location	Date(s)	Hours	Number of Participants	Number of Under-represented people	Method
Presentation	Internet2 CTO Update – Wendy Huntoon	Internet2 Fall Member Meeting Phila, PA	01-04 Oct 2012	1.25	30		Live Webcast
Presentation	Web10G: Meeting the Promise of Web100 – Chris Rapier	Internet2 Fall Member Meeting	01-04 Oct 2012	1.25	10		Live
Panel Session	Regionals Go Above the Net – Michael lambert	Internet2 Fall Member Meeting	01-04 Oct 2012	1.25	20		Live Webcast
Panel Session	R & E Networks: Growth and Sustainability Through Innovation – Wendy Huntoon	Internet2 Fall Member Meeting	01-04 Oct 2012	1.5	30		Live
Workshop	Intro to Parallel Computing and MPI	ERDC Vicksburg, MS	02-03 Oct 2012	16	50		Live Multi-cast

Type	Title	Location	Date(s)	Hours	Number of Participants	Number of Under-represented people	Method
Presentation	PSC Data Supercell – Jason Sommerfield	3ROX GigaPop Meeting Pittsburgh PA	11 Oct 2012	1	20		Live
Presentation & Tour	IT Careers for Pitt-Johnstown MIS Majors – Lynn Layman & J Ray Scott	PSC Pittsburgh PA	10 Oct 2012	2	17	1	Live
Workshop	Virtual workshop on OpenACC	PSC Pittsburgh PA	16-17 Oct 2012	12	140		Live and Webcast
Workshop	OpenMP and Hybrid Programming	ERDC Vicksburg, MS	16-17 Oct 2012	16	50		Live Multi-cast
User Group	Pittsburgh Hadoop User Group Meeting	PSC Pittsburgh PA	17 Oct 2012	2	16		Live
Workshop	MIDAS MISSION Workshop	Arlington, VA	14 Nov 2012	3	50		Live
Workshop	One-day Bioinformatics Workshop – Alex Ropelewski & Hugh Nicholas	Norfolk State Norfolk, VA	11 Oct 2012	4	6	4	Live
Presentation	Summer Bioinformatics Research and Training Opportunities in Pittsburgh – Alex Ropelewski	NC A&T Greensboro NC	16 Oct 2012	1	35	32	Live
Presentation	Accessing Free, Large-scale Computation and Data Resources Through the eXtreme Science and Engineering Discovery Environment (XSEDE)-Alex Ropelelwski	NC A&T	18 Oct 2012	1	8	5	Live
Workshop	One-day workshop on the assembly and analysis of Next Generation Sequencing (NGS) data – Alex Ropelewski	Tennessee State University Nashville NC	24 Oct 2012	8	20	14	Live
Presentation	Summer Bioinformatics Research and Training Opportunities in Pittsburgh	Tennessee State University	22 Oct 2012	1	8	6	Live

Type	Title	Location	Date(s)	Hours	Number of Participants	Number of Under-represented people	Method
Presentation	Accessing Free, Large-scale Computation and Data Resources Through the eXtreme Science and Engineering Discovery Environment (XSEDE) – Alex Ropelewski	Tennessee State University	23 Oct 2012	1	25	15	Live
Lecture	Phylogenetics – Alex Ropelewski	Tennessee State University	22 Oct 2012	1	12	10	Live
Workshop	CMIST – Pallavi Ishwad	Grand Valley State University Allendale MI	25 Oct 2012	8	13	2	Live
Presentations and Panel Session	CMIST & BEST – Pallavi Ishwad	Bioinformatics and Computational Biology Symposium Grand Valley State University	26 Oct 2012	8	25	8	Live
Presentations & Demos	Sherlock: PSC's YarcData uRiKA™ - Nick Nystrom, Deb Nigra & Robin Flaus	SC12 PSC Booth Salt Lake City UT	12-15 Nov 2012	.5	40	5	Live
Presentation	Novel Applications on *Blacklight* – Nick Nystrom & Ralph Roskies	SC12 PSC Booth	12-15 Nov 2012	.5	15		Live
Presentations	Open ACC – John Urbanic	SC12 NVIDIA & PSC Booths	12-15 Nov 2012	.5	15		Live
Presentations	Genomics and Novel Applications on *Blacklight* – Phil Blood & Nick Nystrom	SC12 SGI Theater	12-15 Nov 2012	.5	15	4	Live
Workshop	MATLAB Distributed Computing Server on PSC's *Blacklight*	PSC Pittsburgh PA	27 Nov 2012	3			Live
User Group	Pittsburgh Hadoop User Group Meeting	PSC Pittsburgh PA	28 Nov 2012	2	16		Live
Workshop	*Anton* Training – Phil Blood, Marcela Madrid & Markus Dittrich with Chris Harwell from DESRES	PSC Pittsburgh PA	06 Dec 2012	8	15		Live

Leadership in Programming and Support for Accelerators: On October 16-17, PSC led a large, virtual workshop on OpenACC, a recently-emerged approach for programming GPUs that offers significant advantages in ease of use, rapid programming, performance portability, and code maintainability. Jointly taught by PSC and NVIDIA, this greatly expanded virtual workshop reached 140 participants at 9 institutions in 8 states. Keeneland was used for hands-on exercises. Due to Keeneland's being so new, a limit was set of 100 accounts for hands-on access, with the other students auditing. The course reached capacity very quickly, and another set of institutions is on the waiting list for a follow-on which is scheduled for January 15-16, 2013.

This workshop marks the first time PSC held a multi-site class in hi-definition video. Combining state of the art h.323 technologies of the Tandberg Edge hi-definition video codec system, along with the Internet2 Commons' Cisco MSE 8000 h.323/SIP Multipoint Control Unit, we were able to reach the 140 distributed students, in sparkling detail, enhancing the users' experience of being right there in the room with the teacher.

In conjunction with Cisco's Webex content sharing software, a Jabber server developed at PSC specifically for this workshop, and collaboration with the video services of the National Center for Supercomputing Applications, the workshop production staff also created a broadcast-quality enhanced Video On Demand recording available to future students who weren't able to attend in real-time.

This initial hi-def class offering represents the Center's forward commitment to forging new distance-learning strategies that leverage the Center's vast reserves of high performance programming expertise and experience.

OpenACC workshop participants attended nine sites including PSC (left) and NCSA (right). Instructors were John Urbanic (PSC), visible on the screen at NCSA (right) and Mark Ebersole (NVIDIA), speaking at PSC (left).

Leadership in Hybrid Programming: PSC taught PETTT workshops on *Intro to Parallel Computing and MPI* (October 2-3) and *OpenMP and Hybrid Programming* (October 16-17) at ERDC (Vicksburg, Mississippi) which were broadcast to other DoD sites. *Blacklight* was made available for exercises for workshop participants.

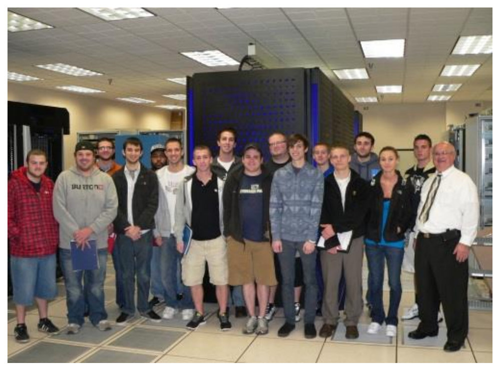
Biomedical Outreach: Education Program Director Pallavi Ishwad continues to lead BEST and CMIST, outreach programs developed by PSC's National Resource for Biomedical Supercomputing (NRBSC). BEST (Better Educators of Science for Tomorrow) is a program that prepares teachers to refocus their teaching strategies towards encouraging students to become aware of emerging and exciting biomedical careers. It provides a high school level bioinformatics curriculum developed by NRBSC and ongoing support for teachers. CMIST (Computational Modules in Science Teaching) brings innovative science tutorials into secondary school classrooms, focusing on integrative computational biology, physiology, and biophysics. In contrast to other teaching tools, CMIST modules include high quality, biologically realistic 3-D animations produced with cutting-edge simulation and visualization software developed at NRBSC.

Ishwad conducted a CMIST Workshop on Thursday, October 25, 2012 at Grand Valley State University where she presented two CMIST modules – "Molecular Transport in Cells: Osmosis and Diffusion" and "Enzymes: Structure & Function". Thirteen high school teachers attended this full day CMIST workshop. She also conducted a meeting of four BEST teachers at PSC on Friday, November 16, 2012 from 8am to 4pm. Participant teachers are in the fourth year of using the BEST curriculum. The agenda was to bring all the BEST minds to one table (Pun intended!) for discussion about classroom experiences using the BEST Bioinformatics curriculum. Many teachers suggested edits to the curriculum incorporating successfully tried classroom exercises. These have now been incorporated into the curriculum.

The teachers decided to create a networking stream to continuously correspond with each other to share best classroom practices throughout the academic school year. All teachers reported a growing popularity of our Bioinformatics course as reflected by increasing enrollments into it.

MATLAB on *Blacklight*: PSC presented a 3-hour MATLAB Distributed Computing Seminar (MDCS) on November 27, 2012 in the Stiles Lecture Hall at PSC. We expect that the availability of MATLAB on *Blacklight* will bring new communities of users into XSEDE. We currently have 44 users registered to use MDCS.

Visitors: On October 10, 2012 Lynn Layman and J Ray Scott hosted a group of 16 students and their professor, Phil Svesnik, from the University of Pittsburgh-Johnstown, for a talk and tour of PSC's machine room. The students were mostly MIS majors. Layman introduced the evening and gave an overview of careers in information technology. Scott gave an overview of high performance computing and the story of high performance computing at PSC for the students. After the talk, Layman and Scott showed them PSC's machine room.



17.6 SP Collaborations

PSC's Josephine Palencia played a major role in bringing the ExTENCI Distributed File System into operation in production mode. See §11.2.

First, Palencia created the Kerberos infrastructure at the University of Florida and then set up the Kerberized Lustre-WAN file system between University of Florida, Fermilab, Florida International University and Florida State University and assisted the partners to get it working. She created a test bed at PSC to make this possible. Once the infrastructure was in place, Palencia worked with Lustre code developers in order to resolve a critical issue with Lustre client instability. Second, the team needed to figure out how to make the security-restrictive Lustre file system usable in a real setting. FIU had a non-Kerberized compute cluster consisting of 200 cores and wanted to use the /extenci Lustre file system. Palencia pushed for a posix-compliant solution to make ExTENCI accessible to all general applications. The team was able to integrate and deploy a hybrid setup with kerberos+lustre+posix-compliant XrootD -- the first successful one of its kind. Third, Palencia made recommendations on how to speed up the production test runs.

17.7 SP-Specific Activities

Patent Issued for Zest: The patent application of PSC staff members Paul Nowoczynski, Nathan Stone, Jared Yanovich and Jason Sommerfield for Zest called "HIGH EFFICIENCY, HIGH PERFORMANCE SYSTEM FOR WRITING DATA FROM APPLICATIONS TO A SAFE FILE SYSTEM" issued as United States Patent No. 8,316,288 on November 20, 2012. Zest is a parallel storage system specifically designed to meet the ever-increasing demands of HPC application checkpointing. Zest differs from traditional parallel filesystems by making use of log-structuring filesystems on the I/O server in combination with opportunistic data placement. Utilizing these techniques, Zest is capable of driving its disks at 90% of peak bandwidth. Read more about Zest at http://quipu.psc.teragrid.org/zest.

External Relations: The work by PSC's National Resource for Biomedical Supercomputing on large scale image registration with Clay Reid's lab at Harvard University was mentioned (p. 295 in the pdf) in a *Nature* article on connectomics in the Oct 11 issue entitled "High-throughput anatomy: Charting the brain's networks" <http://www.nature.com/nature/journal/v490/n7419/full/490293a.html>.

17.8 Publications

D Bourilkov, P Avery, M Cheng, Y Fu, B Kim, J Palencia, R Budden, K Benninger, D Shrum and J Wilgenbusch, "Using virtual Lustre clients on the WAN for analysis of data from high energy physics experiments", 2012, *J. Phys.: Conf. Ser.* **396** 032013 (doi:10.1088/1742-6596/396/3/032013).

S. R. Ribone, V. Leen, M. Madrid, W. Dehaen, D. Daelemans, C. Pannecouque, M. C. Briñón, "Synthesis, biological evaluation and molecular modeling of 4,6-diarylpyrimidines and diarylbenzenes as novel non-nucleosides HIV-1 reverse transcriptase inhibitors", *European Journal of Medicinal Chemistry*, 2012, 58, 485-492.

Tarr, TB; Dittrich, M; Meriney, SD; "Are unreliable release mechanisms conserved from NMJ to CNS?", *Trends in Neurosciences*, Volume 36, Issue 1, January 2013, Pages 14–22.

Troy Wymore and Charles L Brooks III, "From Molecular Phylogenetics to Quantum Chemistry: Discovering Enzyme Design Principles through Computation", *Computational and Structural Biotechnology Journal*, Vol. 2. (http://dx.doi.org/10.5936/csbj.201209018).

17.9 Metrics

17.9.1 Standard User Assistance Metrics

Numbers in Table 1 refer to all tickets handled by the PSC help desk in PSC's local ticket system.

Table 1: Distribution of times to resolution for the 412 tickets that were created as well as resolved between 10/1/2012 and 12/31/2012

Ticket Type	Account issues	File systems	Jobs/batch issues	Login/access issues	Software/ apps	System issues	Other
0-1 hr	0	3	10	0	5	2	2
1-24 hrs	11	8	97	0	18	22	21
1-7 days	12	17	51	1	37	36	16
1-2 wks	1	0	2	0	17	1	5
>2 wks	4	0	2	0	8	1	2

Numbers in Table 2 refer to tickets relating to PSC that were handled in the central XSEDE Ticket System.

Table 2: Distribution of times to resolution

Time to Resolution	account issues	file systems	grid software	jobs/batch queues	login/access issues	mss/data issues	network issues	software /apps	system issues	other
0-1 hr		1			1					
1-24 hr								1		1
1-7 d	1			3	2					1
1-2 wk		1			2			7		
> 2 wk	2	1		7	5	2		8		2
Still Open								2		

17.9.2 SP-specific Metrics

Key system statistics for *Blacklight* for 10/1/2012 to 12/31/2012 are shown in Table 3.

Table 3: Operational Statistics - *Blacklight*		
Number of unplanned outages	6	
Number of planned outages	6	
Total outages	12	
Number of job failures due to system faults	64	
Total time* in period (hours)	4,416.00	100.00%
Scheduled Downtime (hours)	38.83	0.88%
Unscheduled Downtime (hours)	51.25	1.16%
Total Downtime (hours)	90.08	2.04%
Total time available to users (total-downtime)	4,325.92	97.96%
% System Utilization	72.87%	

* On *Blacklight* a node is half the machine. Time values listed are expressed in node hours.

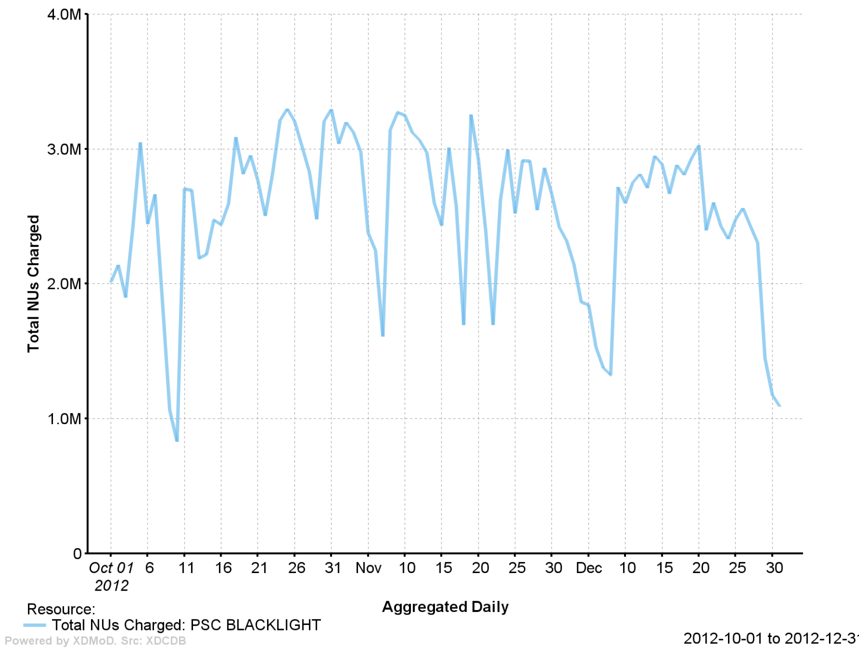
17.9.3 Standard systems metrics

The ten charts of standard system metrics for *Blacklight* on the following five pages were provided by the Technology Audit Services team:

Total NUs Charged by Resource

Service Provider = PSC

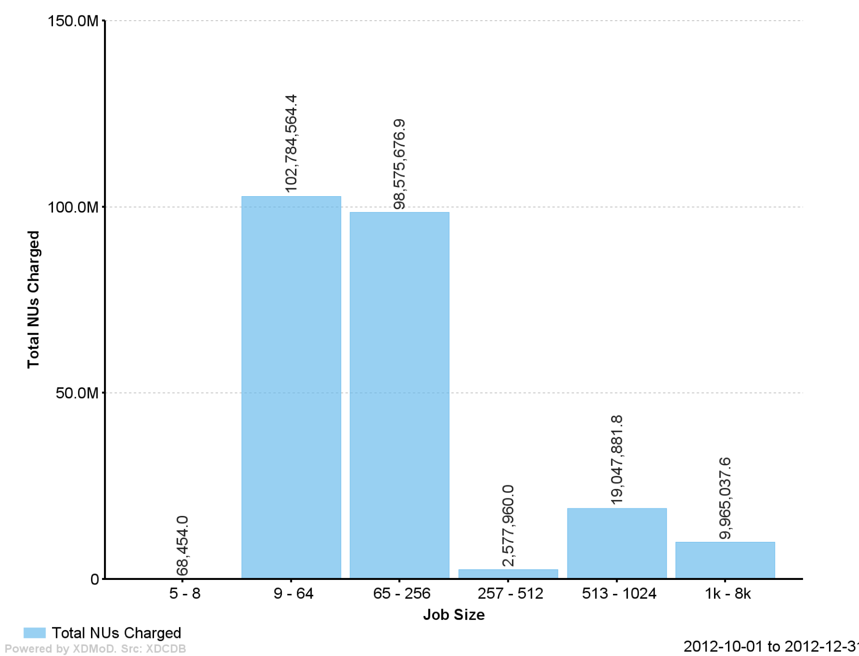
2012-10-01 to 2012-12-31



Total NUs Charged by Job Size

Resource = PSC-BLACKLIGHT

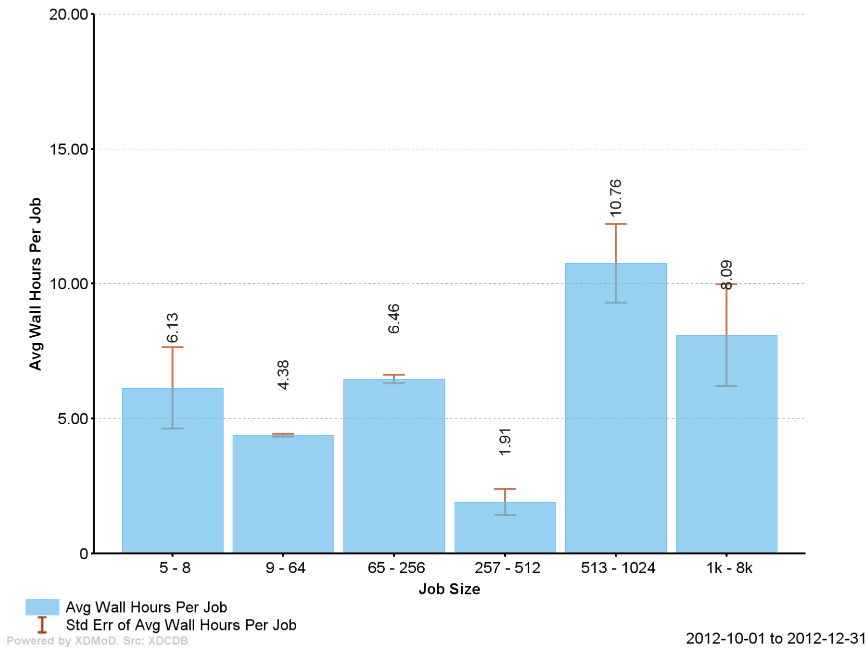
2012-10-01 to 2012-12-31



Avg Wall Hours Per Job by Job Size

Resource = PSC-BLACKLIGHT

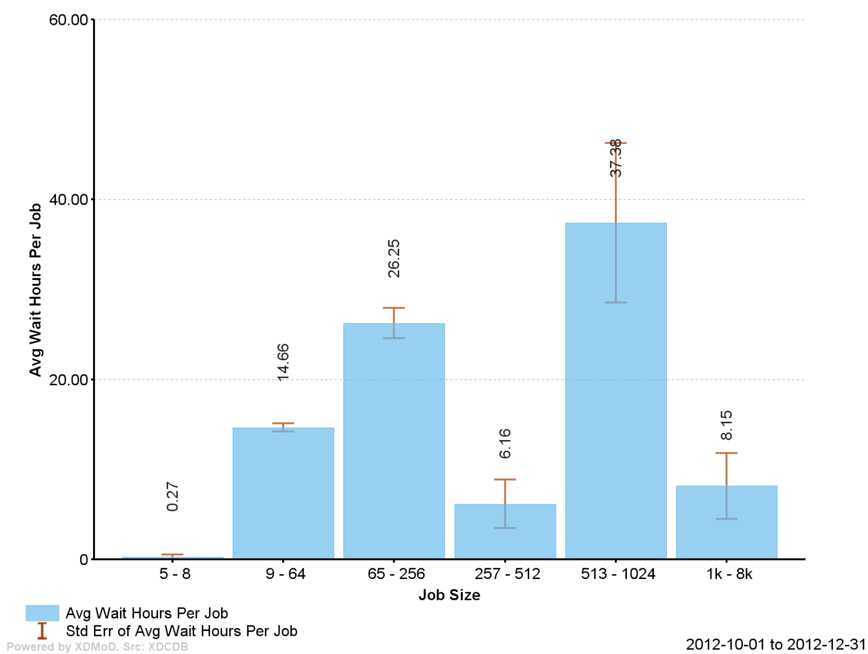
2012-10-01 to 2012-12-31



Avg Wait Hours Per Job by Job Size

Resource = PSC-BLACKLIGHT

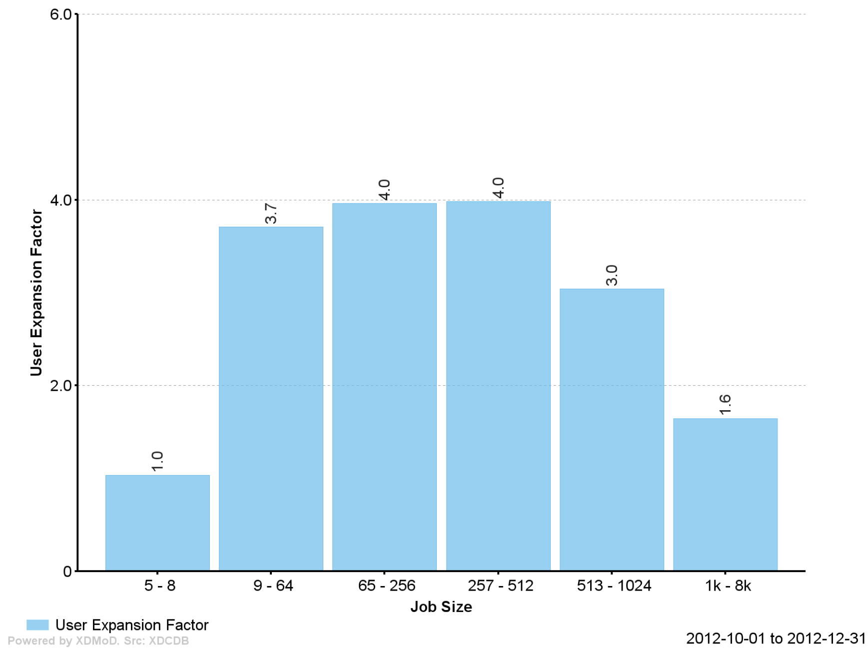
2012-10-01 to 2012-12-31



User Expansion Factor by Job Size

Resource = PSC-BLACKLIGHT

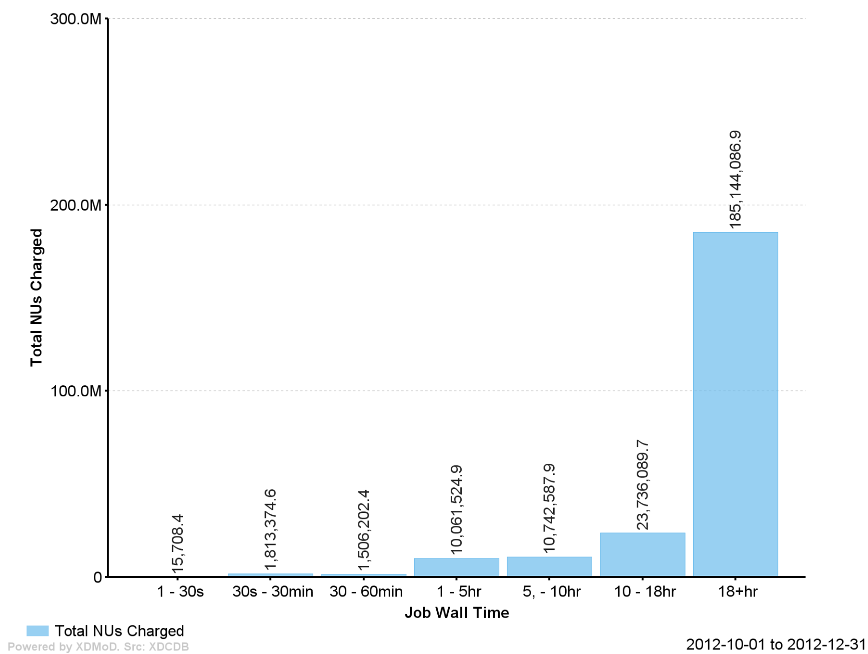
2012-10-01 to 2012-12-31



Total NUs Charged by Job Wall Time

Resource = PSC-BLACKLIGHT

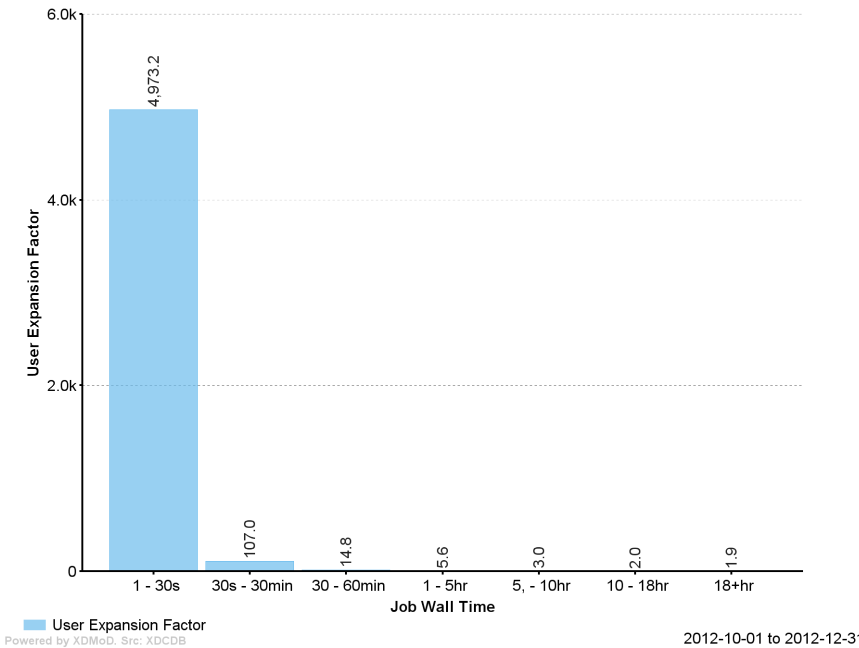
2012-10-01 to 2012-12-31



User Expansion Factor by Job Wall Time

Resource = PSC-BLACKLIGHT -- Service Provider = PSC

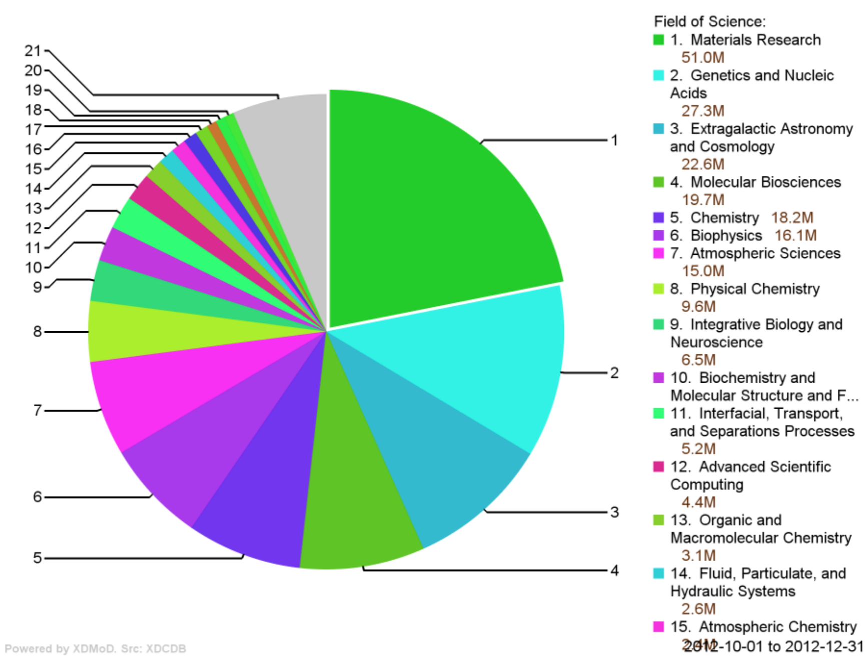
2012-10-01 to 2012-12-31



Total NUs Charged by Field of Science

Resource = PSC-BLACKLIGHT

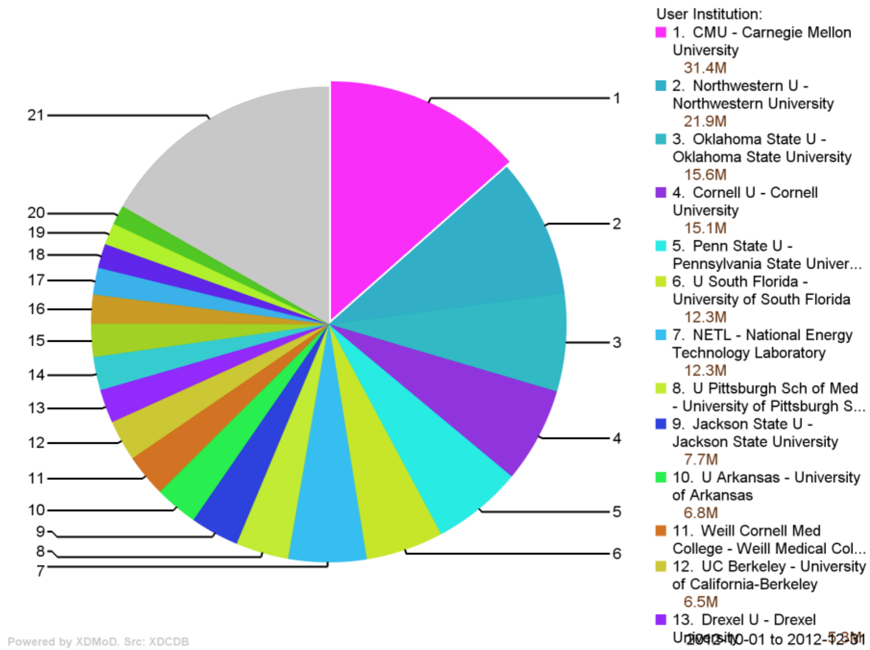
2012-10-01 to 2012-12-31



Total NUs Charged by User Institution

Resource = PSC-BLACKLIGHT

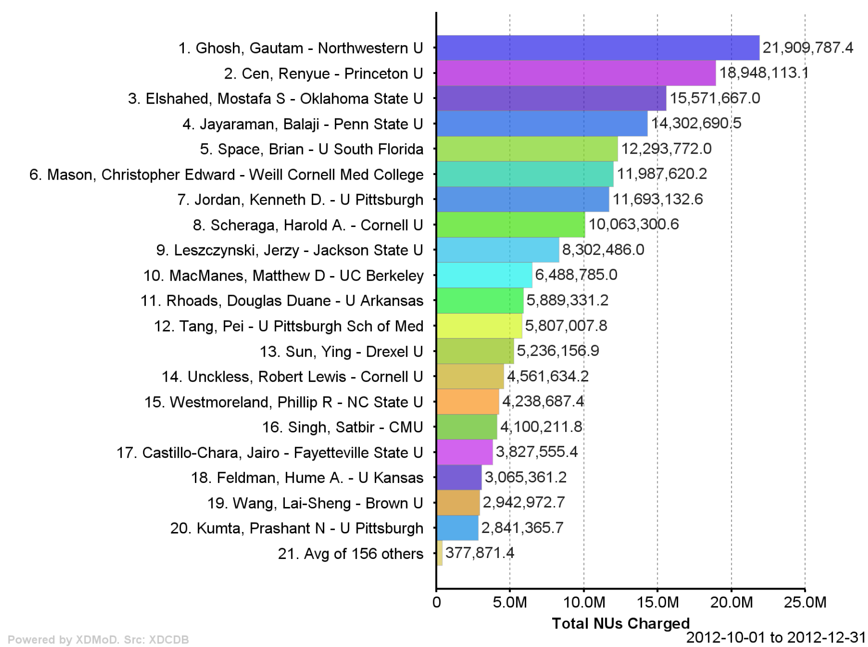
2012-10-01 to 2012-12-31



Total NUs Charged by PI

Resource = PSC-BLACKLIGHT

2012-10-01 to 2012-12-31



18 Purdue University - Service Provider Quarterly Report

18.1 Executive Summary

The Purdue SP provides an HPC cluster (Steele), a high-throughput computing resource (the Purdue Condor pool), and a cloud resource (Wispy) to XSEDE community XSEDE's resource allocation process. The SP operates the systems and provides helpdesk and user support, as well as participate in XSEDE-wide operations, security, software, training and outreach activities. Purdue contributes its expertise in HPC, high-throughput computing, virtualization and science gateway development to assist XSEDE users through training events, tutorials and demonstrations, as well as to the XSEDE ECSS staff on its conference calls and at conferences. These activities are funded by the NSF awards #0503992, #0932251.

Purdue XSEDE resources have supported 145 users (81 projects) from 60 institutions during the reporting quarter. More than 981K total jobs were completed on the Purdue SP resources during this quarter. More than 14 million SUs were consumed by these users and science gateways. Steele has processed a large number of OSG MPI jobs during this quarter, 10 times of what it usually sees in a quarter. Purdue's Condor pool served more than 1.1 million OSG VO jobs during this quarter.

A major system change was made when the SP moved all research cluster user home directories to a newly deployed Isilon extensible storage system. This new system provides a larger default home directory and the potential for large project space for XSEDE users. The maintenance also upgraded many software modules and tools, including schedulers, compilers, and MPIs, with improved reliability and performance.

As a service provider, Purdue continues to support a number of science gateways which provide XSEDE resource-powered scientific simulation and modeling tools, to bridge OSG computation high-throughput HPC (HTHPC) jobs to XSEDE resource, and to develop, deploy virtualization tools to support scientific users of cloud resources as part of the joint TeraGrid-OSG project ExTENCI. Purdue SP staff also supports and contributes to various XSEDE EOT activities and campus information technology community.

18.1.1 *Resource Description*

Steele

The Steele cluster consists of 893 dual quad-core Dell 1950 compute nodes, running Red Hat Enterprise Linux, version 4. Each node thus has 8 64-bit Intel 2.33 GHz E5410 CPUs and either 16 GB or 32 GB of RAM. They are interconnected with either Gigabit Ethernet or InfiniBand. The machine offers access to the 120 TB scratch space. Steele's peak performance is rated at 66.59 TFLOPS. Steele cluster is well suited for a wide range of both serial and parallel jobs. Steele replaced the Purdue Lear cluster and was made available to TG users in May 2008. Its projected useful lifetime is through July 2013. In October 2009, Purdue RP has increased the TG *dedicated* portion of Steele from 22 nodes to nearly 200 nodes (1600 cores). Steele has no effective runtime limit on XSEDE jobs. Additionally, XSEDE users may leverage the larger Steele cluster by utilizing the standby queues with no node limit but subject to 4 or 8 hour runtime limits. Steele is scheduled to retire from XSEDE on July 31, 2013.

Condor Pool

The Purdue Condor pool is a shared resource among the resource owners (academic users at Purdue) and XSEDE/OSG users. Consisting of approximately 50,000 processor cores, the Condor pool is an opportunistic resource which allows Condor jobs access to machines that are not being used by their owners. The Purdue Condor pool is designed for high-throughput computing, and is excellent for parameter sweeps, Monte Carlo simulation, or most any serial application. In addition, some classes of parallel jobs (master-worker) may be run effectively in Condor. 30% of all Condor-usable cycles are available to XSEDE users at a minimum level of service. On average the Purdue Condor pool is able to provide up to 10 million CPU hours to XSEDE users per year.

The Purdue Condor resource, recently named *DiaGrid*, has expanded tremendously from a total of 7700 CPUs at the end of 2007 to its current size of about 50,000 cores (system information shown in Table 1). The Purdue Condor pool consists of nodes from 10 institutions, including Purdue's West Lafayette campus, University of Wisconsin-Madison, University of Nebraska-Lincoln, Indiana University, University of Notre Dame, and a number of Purdue's regional campuses. Memory on most of the compute nodes is 1 GB, 2 GB and 4 GB per core, while a small number of nodes have larger memory (e.g., 10GB per core). With a total of approximately 390 TFLOPS available, the Purdue Condor pool can provide large numbers of cycles in a short amount of time. All shared areas and software packages available on Steele are available on Condor. Available to TeraGrid/XSEDE users since 2006, the Condor pool is self-renewing as old machines in the pool are retired and new ones, e.g., from Purdue's community clusters, added over time. As of this time, Condor pool is scheduled to retire from XSEDE on July 31, 2013.

Table 1: Purdue Condor pool information as of Sept. 31, 2012

System Information	Cores	Total Memory	Local Interconnect	Processor Speed
X86_64 LINUX	49,100	129 TB	IB, 10 Gb or 1 Gb Ethernet	Various (2.1, 2.33, 2.5, 3.2 GHz)
INTEL & X86_64 WINDOWS	409	1.09 TB	1 Gb or 100Mb Ethernet	Various (2.13, 2,66, 3.6GHz)
INTEL LINUX	44	66 GB	1 Gb or 100Mb Ethernet	various
Total	**49,553**	**130 TB**		

Wispy

Purdue's *Wispy* is a special XSEDE resource, a cloud computing platform for research and education use. Wispy consists of 8 64bit, 16-core HP SL230 connected via 1 Gigabit Ethernet network with the capacity of supporting 128 VMs. Wispy runs KVM and the Nimbus cloud software. It provides users with the capability of packaging their applications and operating systems completely inside the Virtual Machine (VM) images, submitting these VMs to run in Wispy with up to 14 CPUs and 32GB of memory each, and have full control over the execution environment. Current usage includes small, instant, on-demand clusters for various tasks and running complicated or prepackaged applications on additional hardware resources.

18.2 Science Highlights

A theoretical study of Dipolar Janus Colloids: Equilibrium Structure and Thermodynamics
PI: Rigberto Hernandez, Physical Chemistry, Georgia Tech

XSEDE resources assist Rigberto Hernandez, professor of chemistry and biochemistry at Georgia Tech, in studies of reactive colloidal systems under various conditions, including the shear rate and the macroscopic boundary conditions used to impose constraints at many scales simultaneously. The results improve models characterizing such systems, which are important in both natural and manmade materials. The results also enhance understanding of how the local, particle-scale interactions within these materials lead to collective or emergent properties.

In addition, Dr. Hernandez's lab is conducting structural and dynamics studies of Janus particles, nanoparticles with a variety of potential uses whose surfaces have two or more distinct physical properties — attractive on one side, repulsive on the other, for example — allowing different types of chemistry to occur on the same particle. The researchers' models go beyond characterizing an abrupt change in properties as a particle rotates to capture the gradual changes during the rotation, like capturing the changes as the sun rises or sets over the rotating Earth. This, likewise, is needed to improve models characterizing the emergence of properties in these systems due to the short-range interactions. Ultimately, the research could inform the design of particles for target properties. As examples, Janus particles might be employed in environment-responsive vehicles for releasing a cargo, such as drugs in the body, in a controlled fashion, as optical probes, or for stabilizing emulsions and foams.

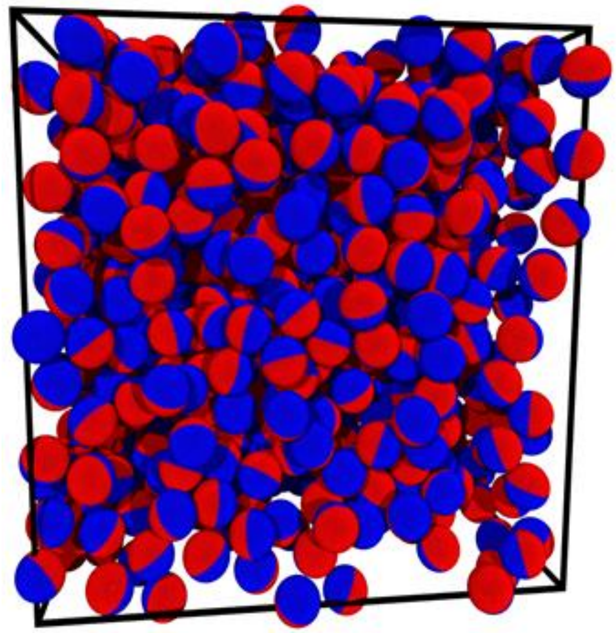


Figure1. Image of simulated dipolar Janus colloids.

Moreover, both sets of simulations shed light on the roles of competing attractive and repulsive regions in the colloid-colloid interaction potential under dynamic conditions.

The work includes development of test-beds for recent advances in the theories and methods of non-equilibrium statistical mechanics concerned with transport processes and chemical reaction rates. The molecular dynamics codes the researchers employ cover many particles, their rotations and their interactions and thus are quite computationally demanding and require both parallel and serial computations. In 2012, Hernandez and his students used 2 million SUs on Purdue's Steele cluster XSEDE resource and over 25,000 hours on the Purdue Condor pool high-throughput XSEDE resource.

Toward a new coarse-grained model for simulations of lipids and peptides
PI: Qiang Cui, Computational Biophysics & Chemistry, University of Wisconsin

Professor Qiang Cui at the University of Wisconsin uses Purdue's Steele cluster and other XSEDE resources for diverse molecular simulation techniques employed by his research group to study proton pumping in biomolecules, energy and signal transduction in bimolecular machines, biomembrane remodeling, binding specificity of transition metal ions to proteins and catalytic promiscuity and specificity — all related to vital protein function in biology and biological membranes. Cui and colleagues are interested in these problems because they are of fundamental biophysical significance and there are biomedical implications as well. Understanding how biological systems transduce energy from one form to another with great efficiency could ultimately inform the development and construction of artificial systems that can accomplish similar tasks, but perhaps work under different conditions, different temperatures or salt concentrations, for instance.

From the biomedical perspective, mutations in proteins involved in bioenergy transduction are often implicated in serious human diseases because alterations in energy production and transduction, whether from external or internal causes, can lead to malfunctions in mitochondria and overproduction of reactive oxygen species, or ROS, chemically reactive molecules that are damaging to cells. Understanding factors that dictate the function of these proteins can broaden strategies to battle relevant diseases, such as cancer and neurodegenerative diseases.

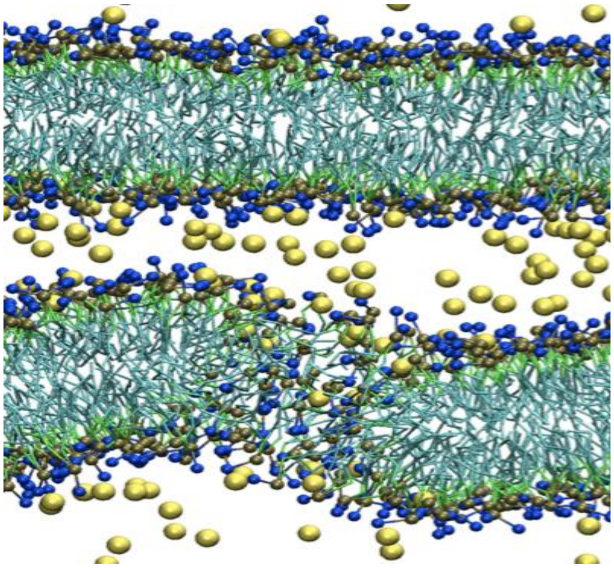


Figure2. A coarse-grained model for biomembrane simulations

Cui's group applies quantum mechanics/molecular mechanics (QM/MM) methods to study enzyme catalytic promiscuity, metal binding selectivity, DNA repair, proton pumping and reactions in bulk water. They also develop and apply coarse-grained models to study peptide and protein interactions that generate morphology changes in biomembranes.

18.3 User-facing Activities

18.3.1 System Activities

The Steele cluster continues to be busy and highly utilized by the XSEDE users during the reporting period. Steele continues to see higher allocation requests than its available cycles for last quarter, and the trend is even higher demand in the November allocation cycle. XSEDE users access Steele through the XSEDE queues, and in addition to the NSF funded portion of the cluster, XSEDE users have access to the entire cluster through its standby queues with a wall clock limit of 4 hours for the jobs. In this manner, XSEDE users typically consumes as high as three times of the cycles allocated for XSEDE on a monthly basis. Figure 3 illustrates the total usage on Steele by XSEDE users since Jan. 2012.

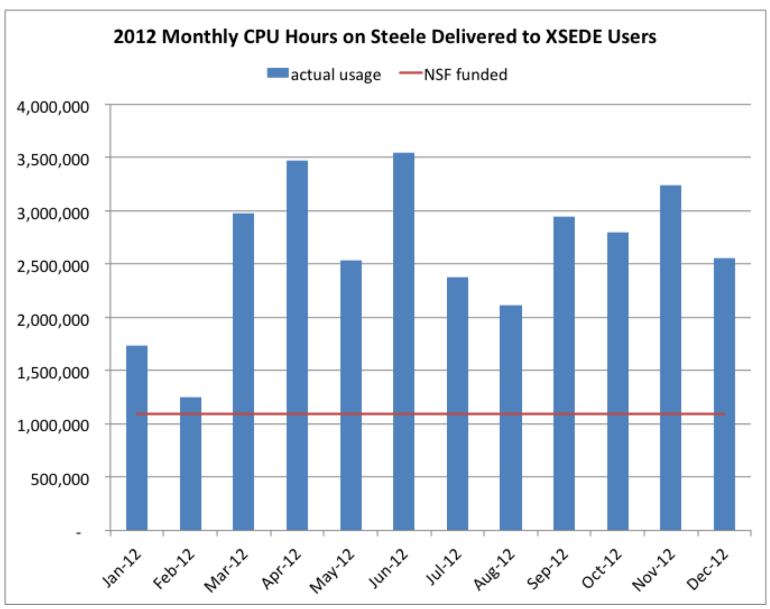


Figure 3. Usage of Steele delivered to XSEDE users, Oct. 2011 – Dec. 2012

The SP had a major scheduled maintenance in

December 2012 when migration of Purdue's research cluster home directories was completed. This migration moved research home directories to the new storage system Isilon deployed for the new Boiler Backpack service (http://www.purdue.edu/boilerbackpack). This upgrade is more than a technology update for the storage hardware, but a solution to provide exciting new capabilities, including a larger default space quota and the removal of file limit quota. The extensibility of the storage offers project space for large data storage in a storage "condo" model.

Also during this downtime, data center upgrades were performed, and maintenance to the research computing network was completed. Lastly, the PBS software on Steele was upgraded to Torque version 4.1 and Moab 7, which will provide for more reliable job management and scheduling. The application software modules provided for use on the Steele were also updated - with many older version of software retired, and all toolchains built with consistent versions of compilers and MPIs - with Intel 13.0.1.117 or PGI 11.8, and OpenMPI 1.6.3. All toolchains built with GCC now use a consistent version of GCC - 4.7.2.

The SP strives to provide the highest level of system availability to its cluster users (see table of uptime percentages at right). There was two unscheduled downtime in October and November related to network and file system access issues. Both were resolved promptly. The December scheduled maintenance on all of Purdue research computing systems lasted 72 hours.

	%Uptime (monthly)		
2012	Condor	Steele	Wispy
Oct	99%	99%	99%
Nov	100%	99%	100%
Dec	90%	90%	90%

18.3.2 Services Activities

Purdue SP provides both helpdesk support and consulting support to XSEDE users. The SP user support staff worked with many XSEDE users during the quarter. Most of the support requests were related to troubleshoot issues. Categories of user issues and requests are summarized in the table in Section 1.9.2.

Purdue's campus champion program staff have identified 10 potential contacts to discuss possible access to XSEDE resources. A few of these are all students in a class that might benefit from access to XSEDE resources. Purdue staff worked with local users by translating into training materials for the larger XSEDE community. They actively participated in the face-to-face working meetings and phone meetings for both the Outreach and Regional Champion groups and worked on various documents for XSEDE12 for these two groups. Purdue staff also investigated potential needs for ECSS assistance for OSG allocations with OSG staff, and provided a list of potential users for ECSS assistance to the ECSS group.

In this quarter, Purdue SP staff identified all current Purdue Condor Pool allocations to determine which ones may benefit from transition to and assistance with using OSG since the Condor Pool is scheduled to retire from XSEDE as of July 31, 2013. The SP also worked with allocations closely through the most recent allocation cycle to make adjustments and recommendations on requests for Steele as Steele is scheduled to retire on July 31, 2013.

18.4 Security

No security incidents were reported during this quarter.

18.5 Education, Outreach, and Training Activities

18.5.1 EOT Events

Type	Title	Location	Date(s)	Hours	Number of Participants	Number of Under-represented people	Method
Tutorial	MATLAB tutorial	West Lafayette, IN	10/11/2012	6	Approx. 110	unknown	Classroom, hands-on
Presentation	"Diagrid - Instant Access to High Throughput Computing", OSG Campus Infrastructure Community Workshop, by Ben Cotton	San Diego, CA (presented remotely)	11/15/2012	1	Approx. 25	unknown	Remotely presented to conference
Tutorial	An introduction to a GUI based R submit tool: SubmitR	West Lafayette,IN	11/28/2012	2	Approx. 35	unknown	Classroom, hands-on

18.5.2 Education

Purdue is offering a new scientific computing class that gives other students the opportunity to build and operate their own mini supercomputer. Purdue SP staff helped design the course based on their several years of experience of coaching undergraduate students in building and tuning clusters at the Supercomputing conferences. Three SP staff members taught a course (EAS 391) with Earth, Atmospheric and Planetary Sciences Professor Michael Baldwin in Fall 2012. Each student in the class assembled his/her own supercomputer, installed an operating system and other system and application software, including a job scheduler and message passing interface, and then worked with the Weather Research and Forecasting Model (WRF), a scientific application used by both weather forecasters and researchers. The students utilized WRF with real weather-related data for central Indiana and cull the data for information, for instance a rainfall projection for a particular day. Throughout most of the semester, the students learned, hands-on, how to efficiently run scientific applications in such fields as environmental modeling and quantum mechanics. At the end of semester, some of these students made up the Purdue's 2012 student team that participated in the Cluster Challenge competition at SC12 and turned in another strong finish.

18.6 SP Collaborations

The SP staffs continue to work with an USDA funded large collaborative project (USDA-NIFA no. 2011-68002-30220), an integrated research and extension project working to improve farm resilience and profitability in the North Central Region by transforming existing climate information into usable knowledge for the agricultural community. The overall purpose of the project is to develop decision support tools for use in understanding the potential impact of climate change on the production of maize (corn) in the region. The researchers in this project are conducting modeling and data synthesis which often require long runs on resources such as those available on XSEDE and high performance data storage. The SP staff is assisting the research group to investigate how to make the large number of simulation runs manageable by designing workflows, identifying appropriate resources, as well as assisting with data processing tasks. 20 of the desired 30 years of gridded simulation data have been created. In the last three months, the SP staff has also been involved in developing web enabled decision support tools based on a minimum of 30 years of climate data for the region including min and max temperature, rainfall, growing degree days and county yield data.

Purdue RP continues to provide its 50,000 processor pool to OSG user community, and supporting the OSG MPI (high-throughput HPC) jobs on Steele where 8-core parallel OSG jobs flow to the XSEDE Steele. In this quarter, 82,137 OSG MPI jobs ran and consumed 62,011 CPU hours on Steele. More than 1.1 million jobs from various OSG VOs consumed a total of approximately 3.7 million processor hours in Purdue's Condor pool during this quarter.

18.7 SP-Specific Activities

The Purdue SP staff continue to assist with CI development and deployment activities for the WaterHUB project (funded by NSF CI-TEAM program). One important tool, the SWATShare, powered by XSEDE resources (Steele and Condor pool), was released in December. This tool enables users to upload, execute, analyze and share SWAT (Soil and Water Assessment Tool) models in a GIS-enabled online environment. We tested and integrated SWAT 2009 into the modeling environment, improved the GIS map model view interface, added a comprehensive set of model metadata, and completed the online visualization functions for model output. The SP staff also improved the user's workflow by refining the upload mechanism, as well as providing an updated user manual. SP staff are currently working with a faculty member at University of North Carolina who will use WaterHUB to teach a class in spring 2013.

In support of the IsoMAP project (funded by NSF ABI program), the SP staff performed a major, site-wide database update. The update included new data and data sources for both the vector and raster data collections. Vector data were updated to include global isotope monitoring data through 2009 via collaboration with the IAEA (International Atomic Energy Agency). Raster data collections were updated to include the latest version of the CRU (TS 3.1) climate layers and high resolution PRISM data. A new vapor pressure variable from the CRU dataset was enabled to run geostatistical models for precipitation isotope as well. These updates significantly increased the capacity in support of high-resolution, spatiotemporal water isotope mapping. The design and implementation of a new plant water isotope application is also under way.

The Purdue SP is wrapping up the Community Earth System Model (CESM) science gateway project in collaboration with NCAR and NOAA teams. This gateway integrates online modeling using the latest CESM codes, comprehensive metadata generation, data publishing (to Earth System Grid at NCAR), post processing, and NOAA-PMEL's Live Access Server to visualize, subset and access in different ways of geo-referenced scientific data. To prepare for the production release of the portal, LAS was installed on the Purdue ESG data node and is being integrated into the model output processing pipeline. With the upcoming retirement of Steele cluster, the Purdue SP also submitted an XD renewal proposal and received a new allocation on Trestles. The Purdue SP will work on the migration of the CESM portal to submit jobs to Trestles in the first quarter of 2013.

18.8 Publications

User publications:

Matthew C. Hagy and R. Hernandez, "Dynamical Simulation of Dipolar Janus Colloids: Equilibrium Structure and Thermodynamics," J. Chem. Phys. 137(4): 044505 (2012). (doi:10.1063/1.4737432).

G. Ozer, S. Quirk and R. Hernandez, "The energetics of decaalanine stretching in water obtained by adaptive steered molecular dynamics simulations," J. Chem. Theory Comput. 8, 4837-4844 (2012). (doi:10.1021/ct300709u).

G. Ozer, S. Quirk and R. Hernandez, "Adaptive steered molecular dynamics: Validation of the selection criterion and benchmarking energetics in vacuum," J. Chem. Phys. 136, 215104 (2012). (doi:10.1063/1.4725183).

Catalysis induced by molecular self-assembly: insights from computer simulation, J. Mondal, X. Zhu, Q. Cui and A. Yethira j, J. Phys. Chem. B 116, 491-495 (2012)

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Staff publications:

Ganeshchandra Mallya; Lan Zhao; Xiaohui C. Song; Dev Niyogi; Rao S. Govindaraju. “On the 2012 Drought in Midwest, USA," Forum article. Accepted by the Journal of Hydrologic Engineering. Dec. 2012.

18.9 Metrics

18.9.1 Standard User Assistance Metrics

Purdue SP ticket resolution times by category from XSEDE ticket system:

Time to Resolution	account issues	file systems	grid software	jobs/batch queues	login/access issues	mss/data issues	network issues	software/apps	system issues	other
0-1 hr										
1-24 hr	1									1
1-7 d	3			8	2			2	13	7
1-2 wk		1		1	1			1	3	1
> 2 wk		1		4	2			1	5	2
Still Open										

18.9.2 SP-specific Metrics

Purdue SP ticket summary:

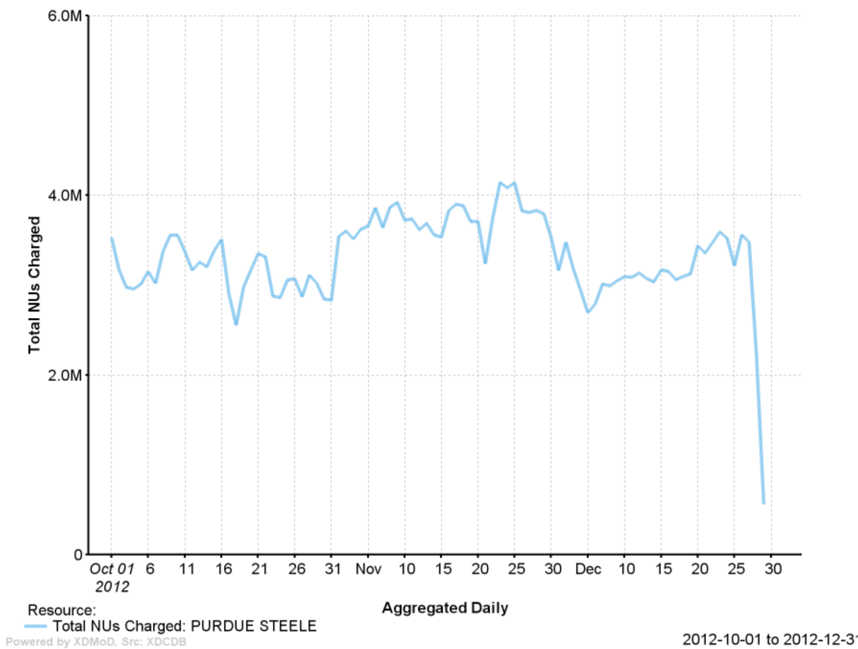
Category	Tickets Received	Tickets Closed	Activities
account issues	7	7	custom group creation, training accounts, shell change
csa requests	0	0	
file systems	5	5	quota increases, find scratch, shared filesystem questions
gateways	0	0	
gpfs-wan	0	0	
grid software	2	2	ifort compiler
inca test reports	8	8	MDS stale providers and failures, host certificates expired
jobs / batch queues	24	24	SU question, queue choices, long wait time, errors with modules, qstat errors, obtaining high throughput on condor, multiple serial program execution
login / access issues	7	7	shell change, unable to login, password questions, direct ssh
mss / data issues	1	1	SFTP transfer error
network issues	0	0	
other	2	2	change login shell and quota increase
refund request	0	0	
reservation request	0	0	
security	0	0	
software / apps	7	7	matlab on steele, using R, MPI/OpenMP issue, java, using numpy
system issues	17	17	stale MDS providers, load on login node, slow compute nodes on steele
workshops	0	0	
TOTAL	80	80	

18.9.3 Standard systems metrics

PURDUE-STEELE Quarterly Report

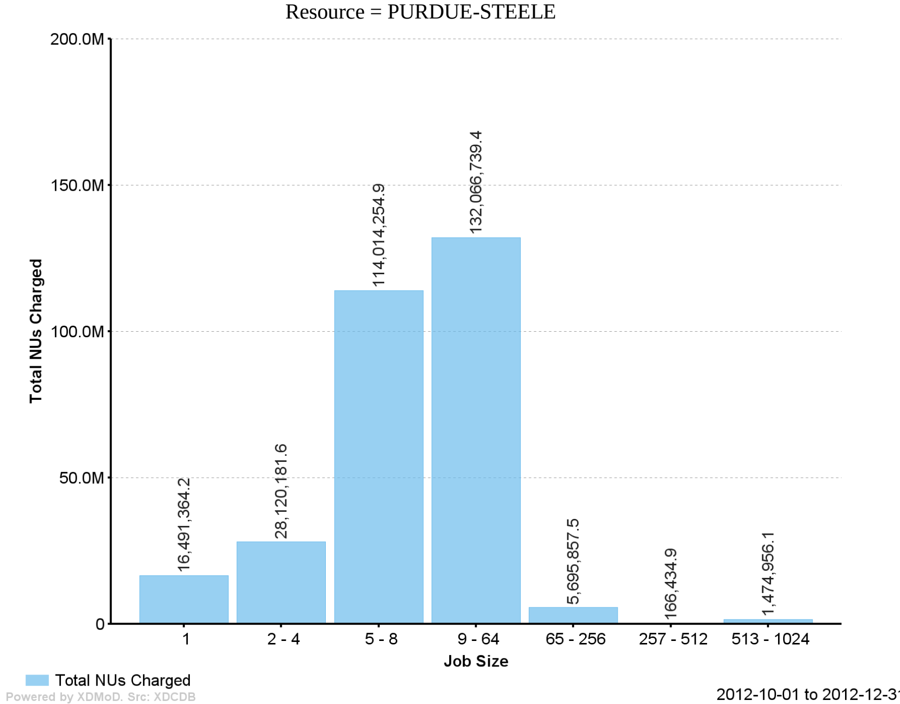
Total NUs Charged by Resource

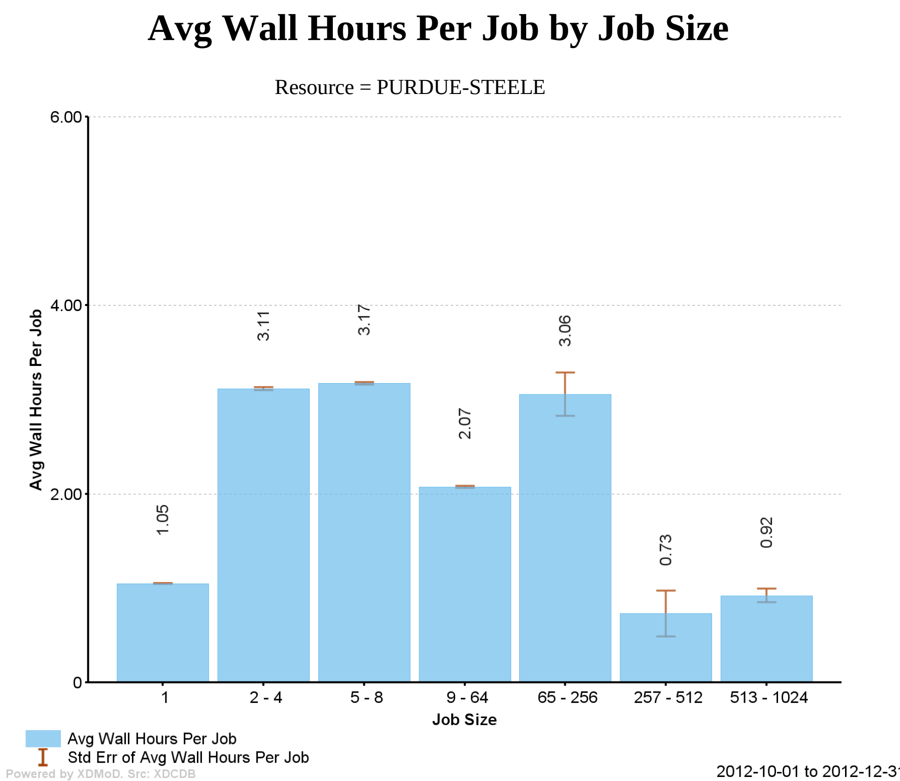
Service Provider = PURDUE

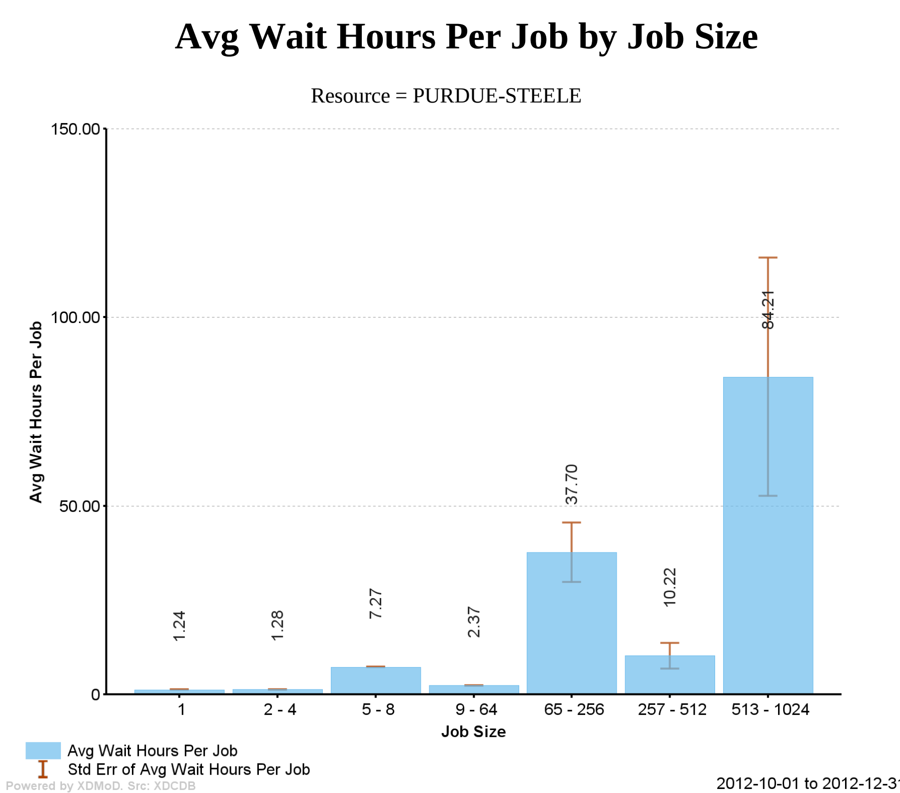


Total NUs Charged by Job Size

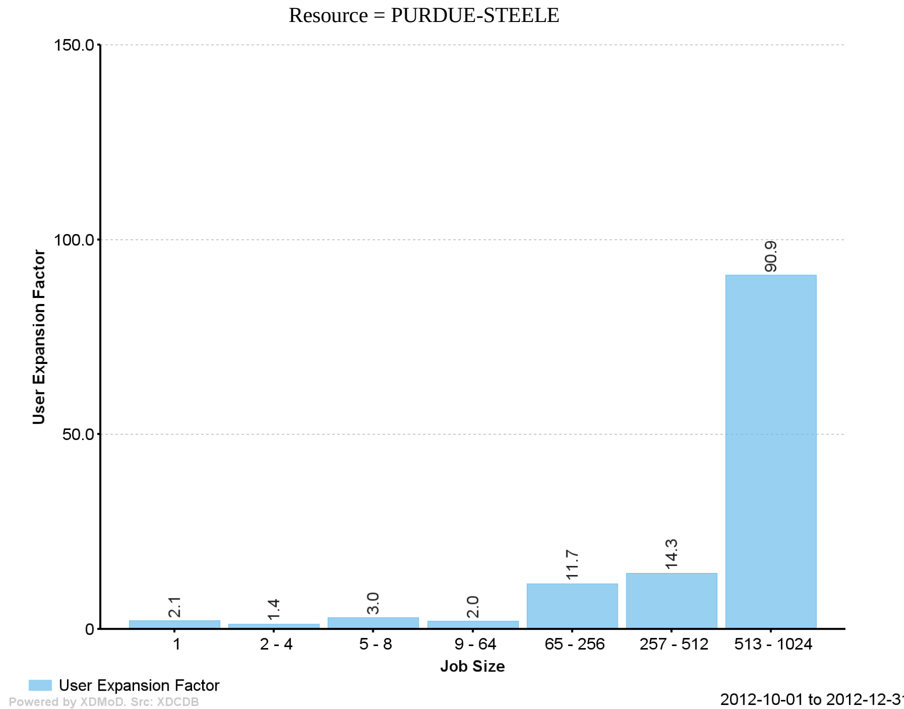
Resource = PURDUE-STEELE



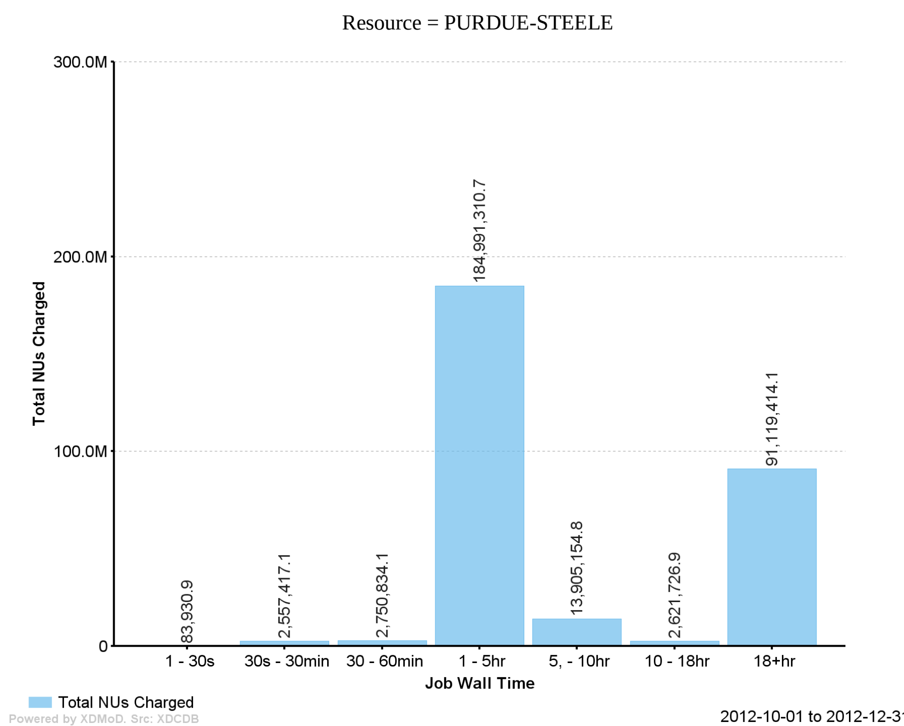

Avg Wall Hours Per Job by Job Size
Resource = PURDUE-STEELE
6.00
4.00
2.00
0
Avg Wall Hours Per Job
1.05
3.11
3.17
2.07
3.06
0.73
0.92
1
2 - 4
5 - 8
9 - 64
65 - 256
257 - 512
513 - 1024
Job Size
Avg Wall Hours Per Job
Std Err of Avg Wall Hours Per Job
Powered by XDMoD. Src: XDCDB
2012-10-01 to 2012-12-31


Avg Wait Hours Per Job by Job Size
Resource = PURDUE-STEELE
150.00
100.00
50.00
0
Avg Wait Hours Per Job
1.24
1.28
7.27
2.37
37.70
10.22
84.21
1
2 - 4
5 - 8
9 - 64
65 - 256
257 - 512
513 - 1024
Job Size
Avg Wait Hours Per Job
Std Err of Avg Wait Hours Per Job
Powered by XDMoD. Src: XDCDB
2012-10-01 to 2012-12-31

User Expansion Factor by Job Size

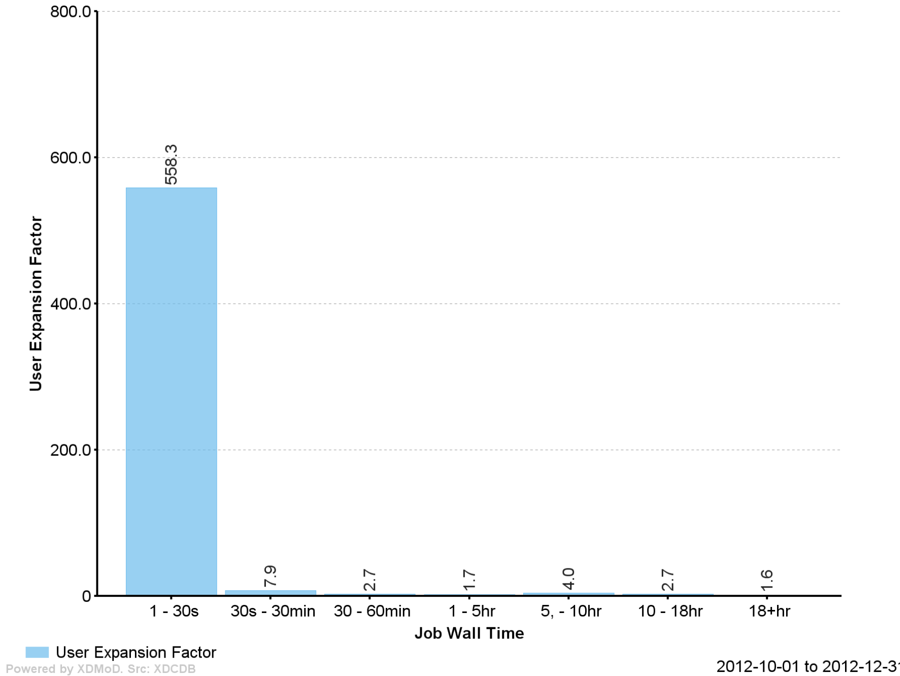


Total NUs Charged by Job Wall Time



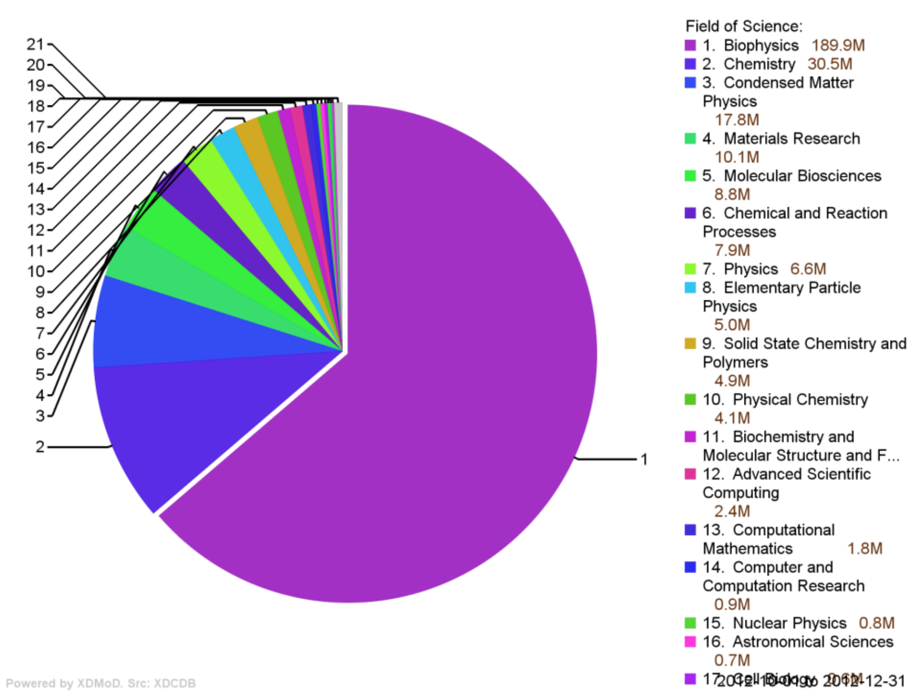
User Expansion Factor by Job Wall Time

Resource = PURDUE-STEELE -- Service Provider = PURDUE



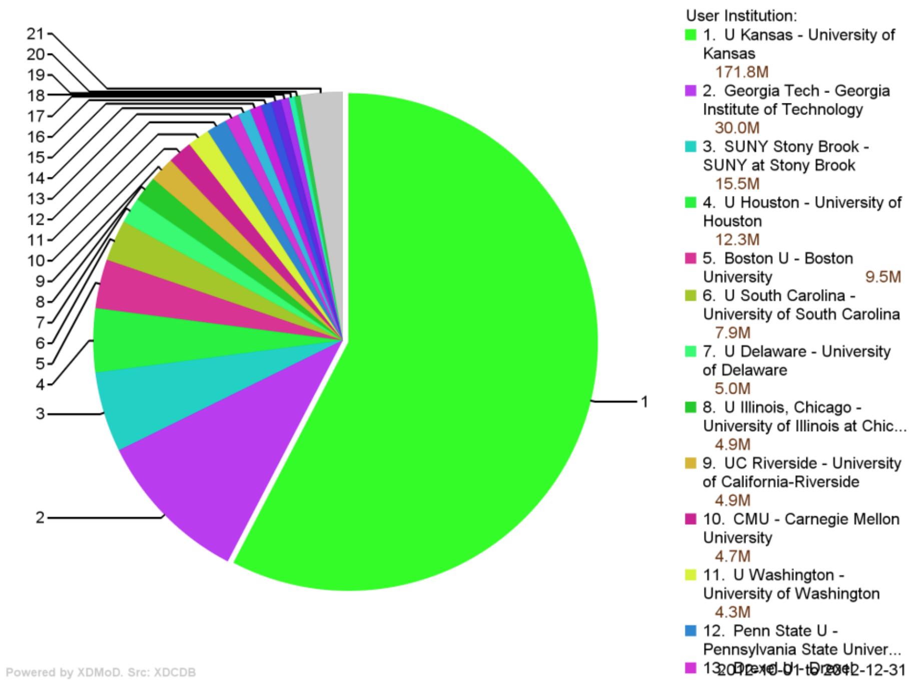
Total NUs Charged by Field of Science

Resource = PURDUE-STEELE



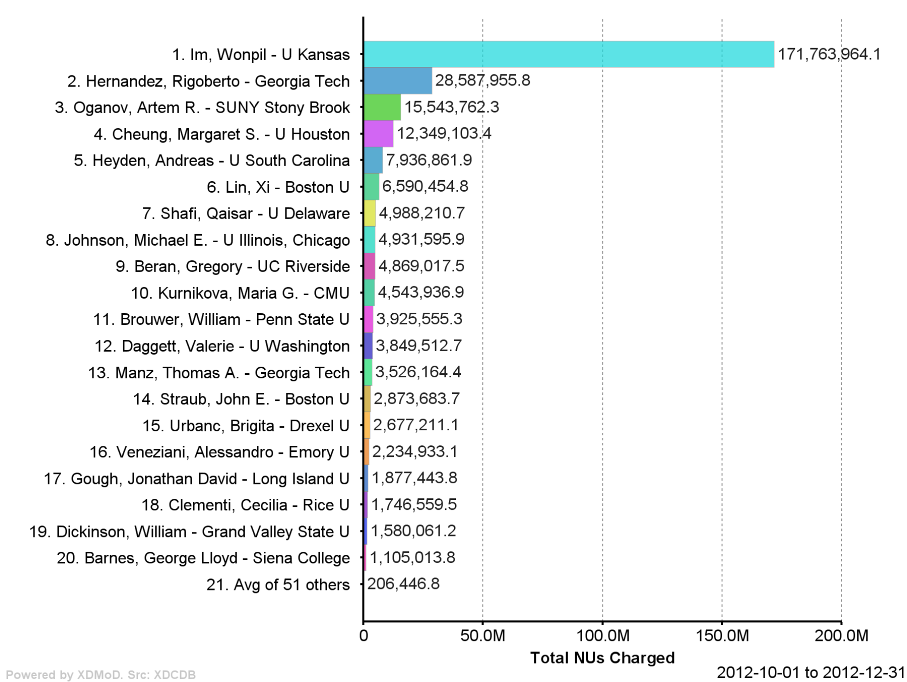
Total NUs Charged by User Institution

Resource = PURDUE-STEELE



Total NUs Charged by PI

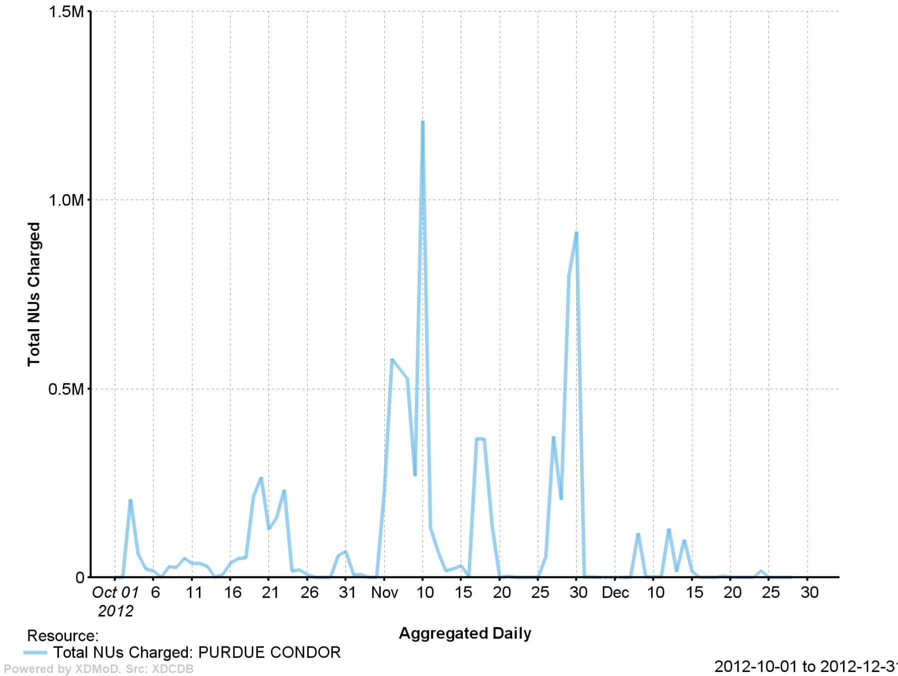
Resource = PURDUE-STEELE



PURDUE-CONDOR Quarterly Report

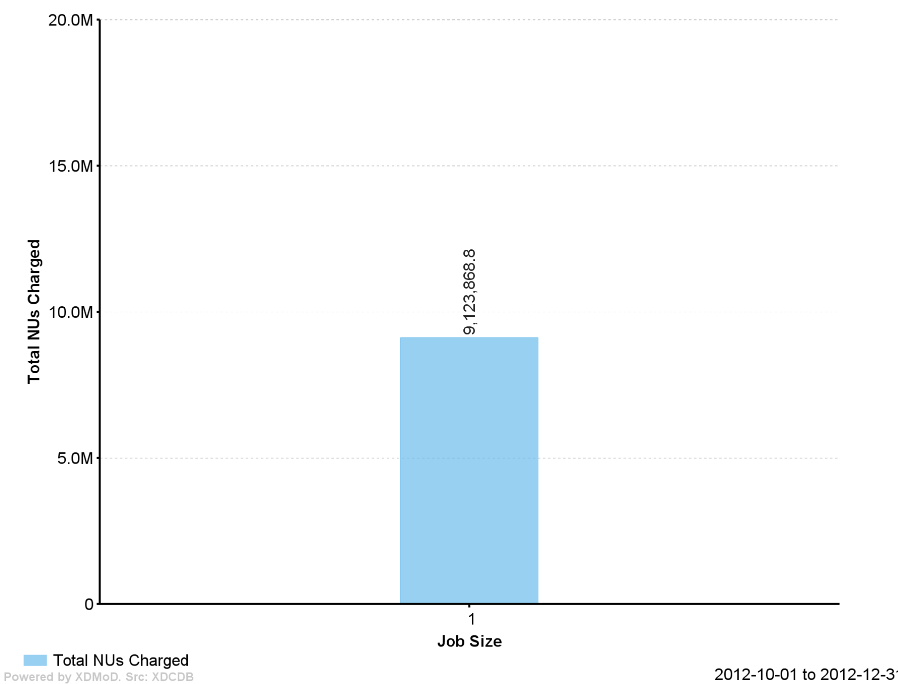
Total NUs Charged by Resource

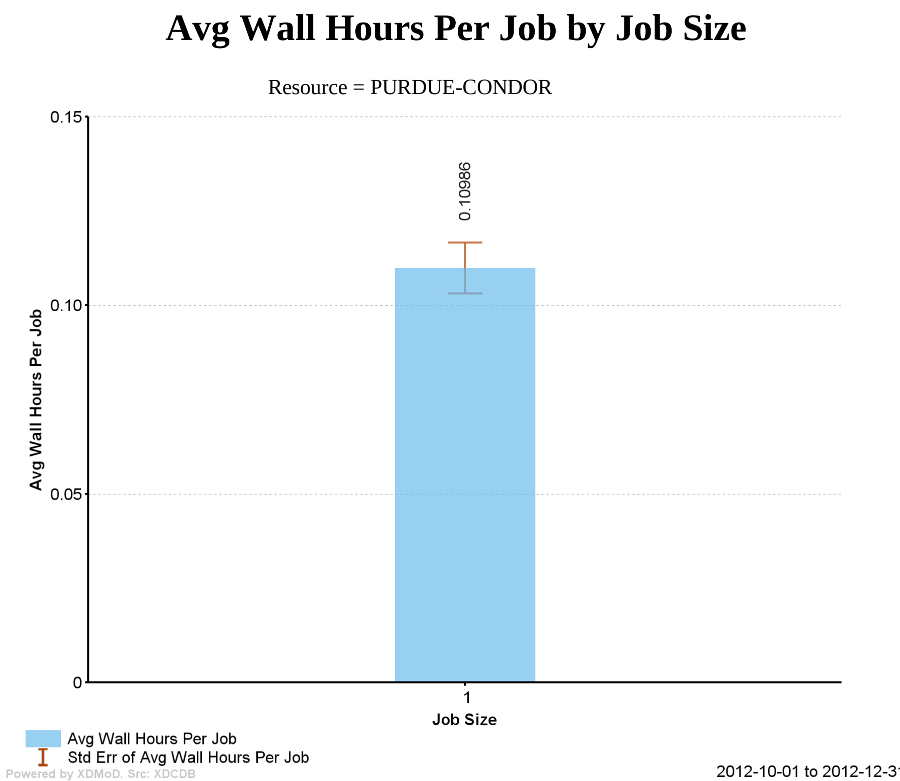
Service Provider = PURDUE

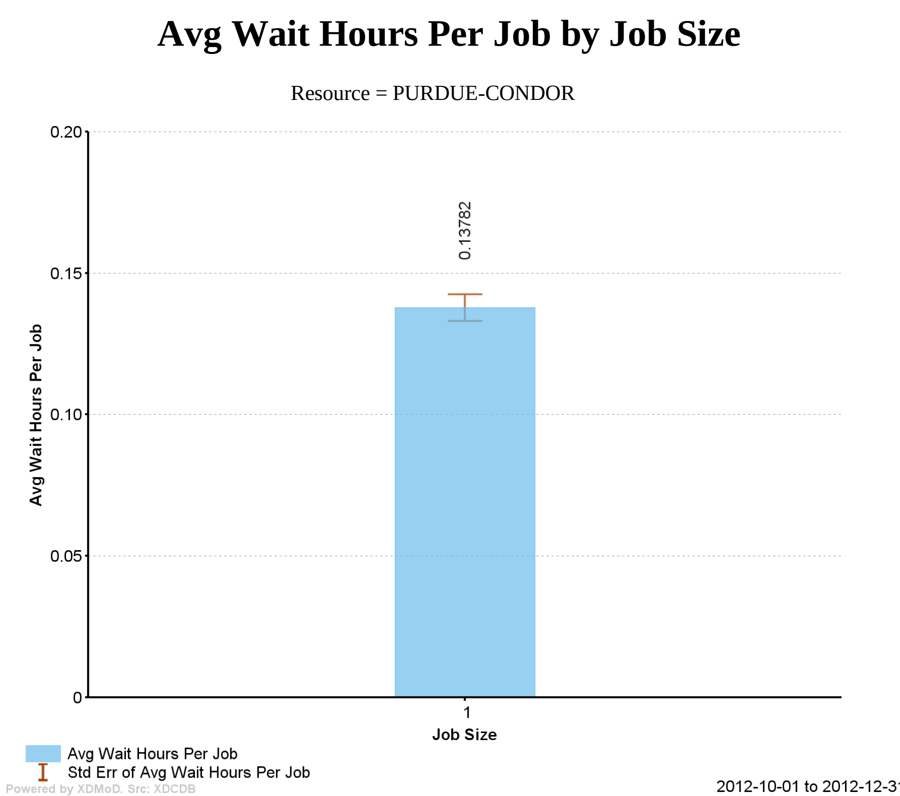


Total NUs Charged by Job Size

Resource = PURDUE-CONDOR

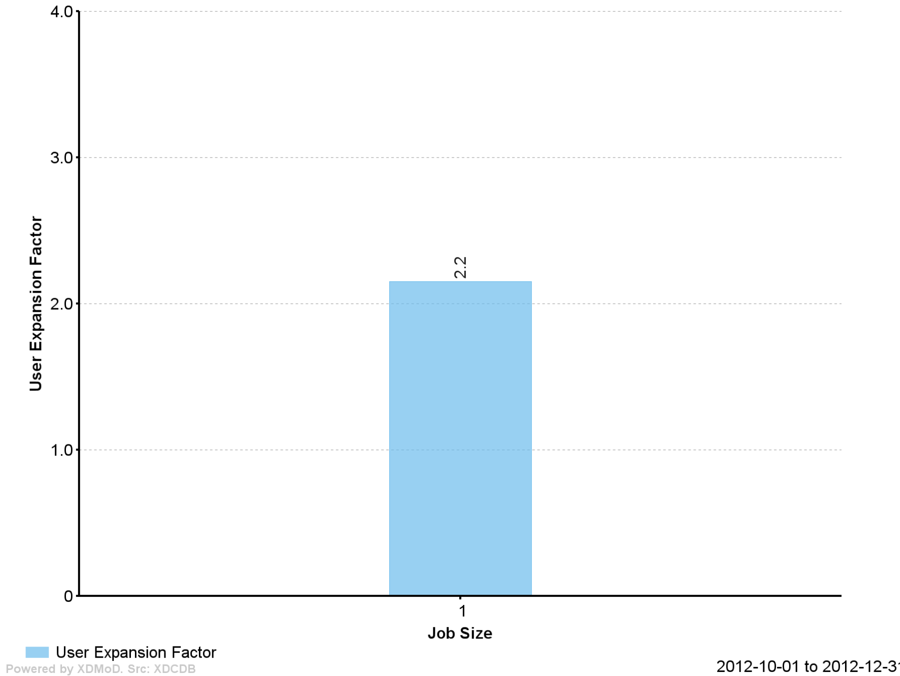



Avg Wall Hours Per Job by Job Size
Resource = PURDUE-CONDOR
0.15
0.10
0.05
0
0.10986
Avg Wall Hours Per Job
1
Job Size
Avg Wall Hours Per Job
Std Err of Avg Wall Hours Per Job
Powered by XDMoD. Src: XDCDB
2012-10-01 to 2012-12-31


Avg Wait Hours Per Job by Job Size
Resource = PURDUE-CONDOR
0.20
0.15
0.10
0.05
0
0.13782
Avg Wait Hours Per Job
1
Job Size
Avg Wait Hours Per Job
Std Err of Avg Wait Hours Per Job
Powered by XDMoD. Src: XDCDB
2012-10-01 to 2012-12-31

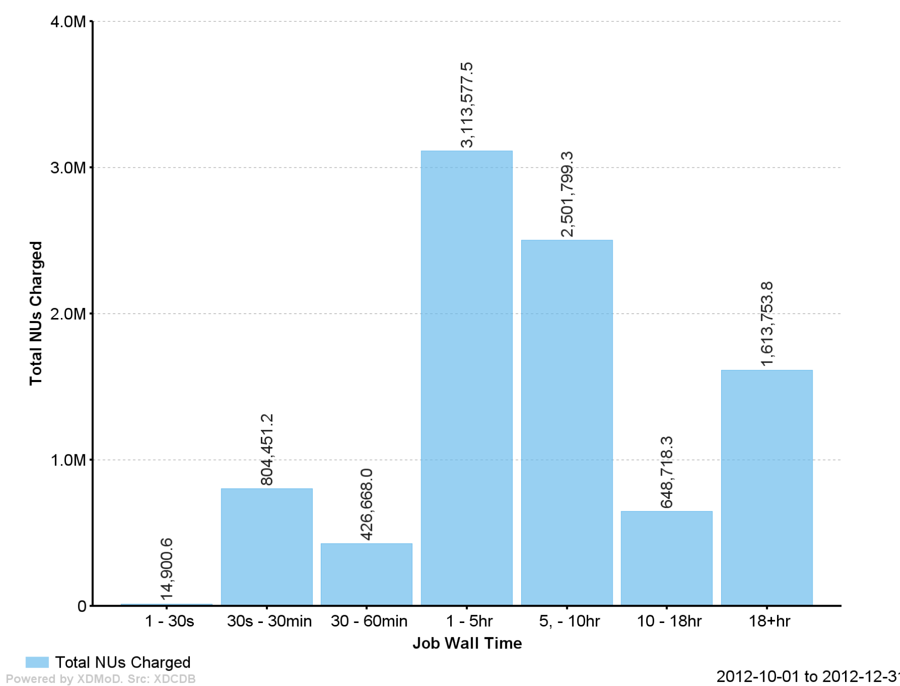
User Expansion Factor by Job Size

Resource = PURDUE-CONDOR



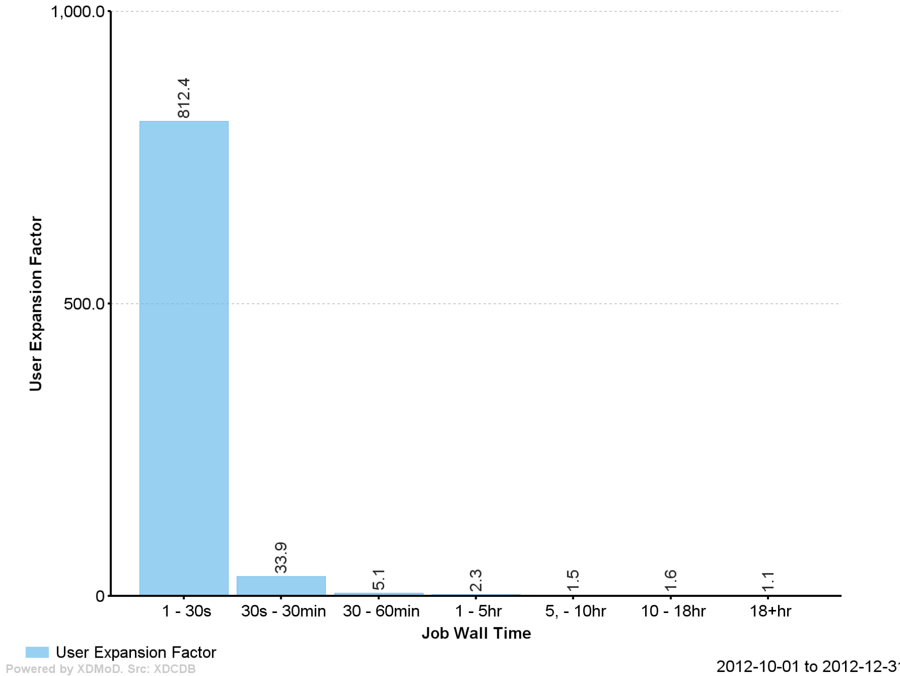
Total NUs Charged by Job Wall Time

Resource = PURDUE-CONDOR



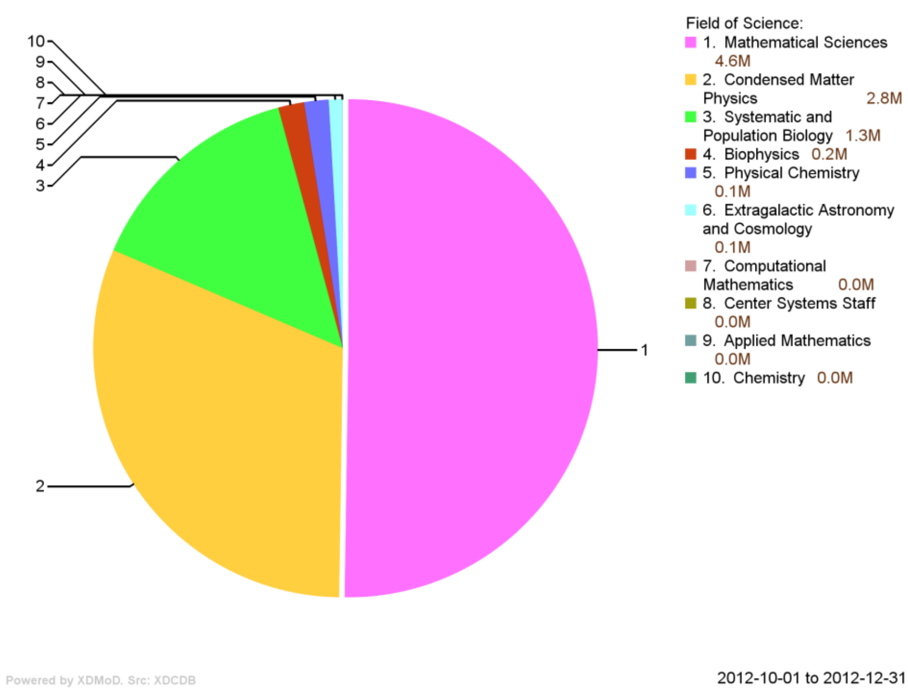
User Expansion Factor by Job Wall Time

Resource = PURDUE-CONDOR -- Service Provider = PURDUE



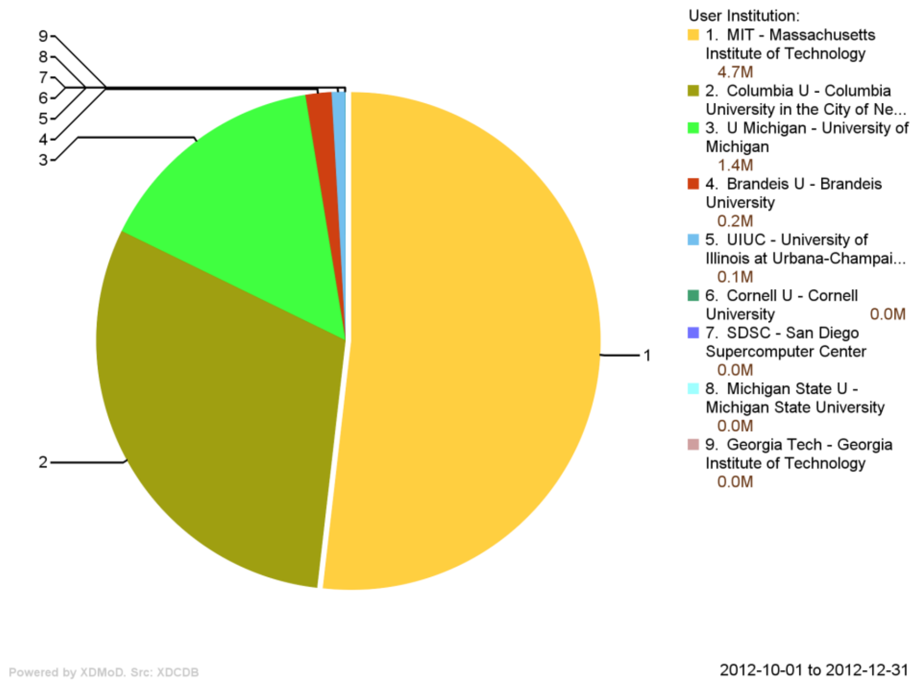
Total NUs Charged by Field of Science

Resource = PURDUE-CONDOR



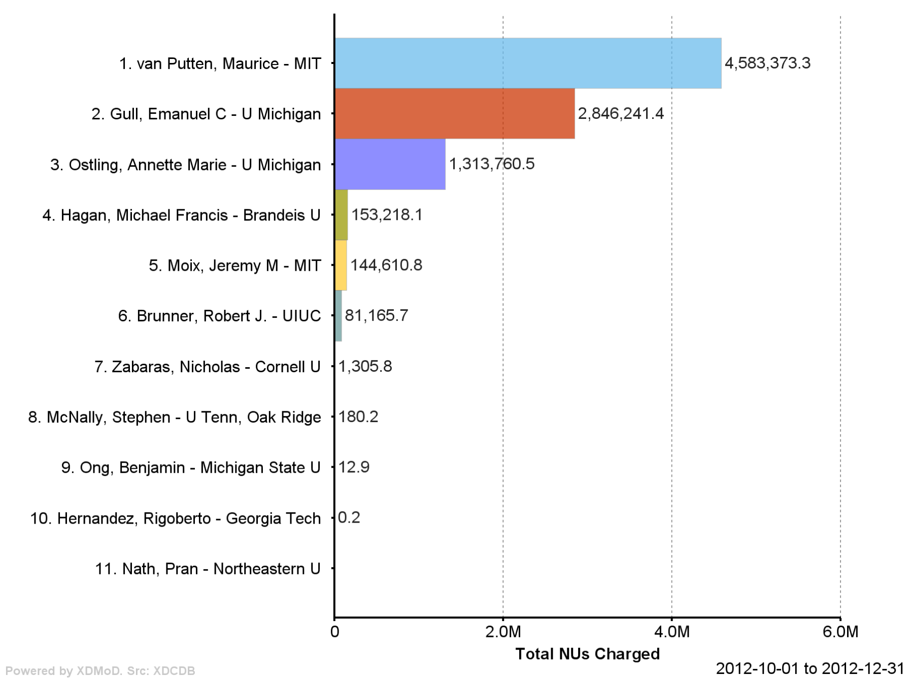
Total NUs Charged by User Institution

Resource = PURDUE-CONDOR



Total NUs Charged by PI

Resource = PURDUE-CONDOR



19 San Diego Supercomputer Center (SDSC) Service Provider Quarterly Report

19.1 Executive Summary

Gordon, which entered production XSEDE operations in Q1, 2012, completed its fourth quarter of operations during the reporting period. Gordon was conceived and deployed as the first XSEDE system to address challenges of data intensive computing. The use of massive amounts of flash memory, large memory nodes, and a high performance parallel file system are proving useful to researchers in a wide range of domains. Startup requests by users who are interested in exploring these features are increasing as are full XRAC requests. 28M SU's (78% of the available cycles) were awarded for a January 1, 2012 start date. *Gordon* also hosted jobs for the CIPRES and GRIDCHEM gateways.

Trestles has now completed two years of production and is highly successful in its objectives to support the modest-scale/gateway user community, with a focus on user productivity and fast turnaround. The system is well over-requested in the allocation process, and is hosting additional gateways beyond the very large CIPRES gateway. The system utilization remains reasonably high while still maintaining our primary objective of short wait times and low expansion factors. Based on financial projections, we have committed to extend the operational life of Trestles at least through June 2014 (was originally December 2013).

SDSC delivered two XSEDE-wide trainings during the reporting period: Intro to Scientific Visualization and Remote Visualization on Gordon (98 attendees); and Introduction to Predictive Analytics for Big Data (120 attendees). Both of these were part of SDSC's thrust to provide training in areas relevant to data-intensive area.

SDSC continued with the project storage pilot project, having allocated more than half of the 400TB of initial project storage. This resource will grow by another 2 PB in 2013Q1 as part of the *Gordon* delivery by Appro. The additional capacity will be used for non-purged, interim storage. SDSC will be offering this resource to XSEDE users through the Storage Allocations process which is currently being developed.

It was announced just after SC'12 that Cray had acquired Appro. SDSC leadership met with the CEO's of both companies and they reiterated their support for SDSC's systems, both of which are Appro clusters. Thus no changes are anticipated to the service levels for these systems.

19.1.1 Resource Descriptions

Gordon

Gordon is a dedicated XSEDE cluster designed by Appro and SDSC consisting of 1024 compute nodes and 64 I/O nodes. Each compute node contains two 8-core 2.6 GHz Intel EM64T Xeon E5 (Sandy Bridge) processors and 64 GB of DDR3-1333 memory. The I/O nodes each contain two 6-core 2.67 GHz Intel X5650 (Westmere) processors, 48 GB of DDR3-1333 memory, and sixteen 300 GB Intel 710 solid state drives. The network topology is a 4x4x4 3D torus with adjacent switches connected by three 4x QDR InfiniBand links (120 Gbit/s). Compute nodes (16 per switch) and I/O nodes (1 per switch) are connected to the switches by 4x QDR (40 Gbit/s). The theoretical peak performance of Gordon is 341 TFlop/s.

Trestles

Trestles is a dedicated XSEDE cluster designed by Appro and SDSC consisting of 324 compute nodes. Each compute node contains four sockets, each with an 8-core 2.4 GHz AMD Magny-

Cours processor, for a total of 32 cores per node and 10,368 total cores for the system. Each node has 64 GB of DDR3 RAM, with a theoretical memory bandwidth of 171 GB/s. The compute nodes are connected via QDR InfiniBand interconnect, fat tree topology, with each link capable of 8 GB/s (bidirectional). Trestles has a theoretical peak performance of 100 TFlop/s.

19.2 Science Highlights

Novel Studies of Gene Regulation in Brain Development May Mean New Treatment of Mental Disorders

A team of researchers at UC San Diego and the Institut Pasteur, Paris has come up with a novel way to describe a time-dependent brain development based on coherent–gene-groups (CGGs) and transcription-factors (TFs) hierarchy. The findings could lead to new drug designs for mental disorders such as autism-spectrum disorders (ASD) and schizophrenia.

In the paper, published November 22 as an online-first publication in the journal *Genes, Brain and Behavior*, the researchers identified the hierarchical tree of CGG–TF networks that determine the patterns of genes expressed during brain development and found that some "master transcription factors" at the top level of the hierarchy regulated the expression of a significant number of gene groups.

Instead of a taking the approach that a single gene creates a single response, researchers used contemporary methods of data analysis and SDSC's *Gordon* supercomputer to identify CGGs responsible for brain development which can be affected for treatment of mental disorders. Please see http://www.sdsc.edu/News%20Items/PR113012_brain.html for the full press release.

Human Brain, Internet, and Cosmology: Similar Laws at Work?

The structure of the universe and the laws that govern its growth may be more similar than previously thought to the structure and growth of the human brain and other complex networks, such as the Internet or a social network of trust relationships between people, according to a new paper published in the science journal *Nature's Scientific Reports*.

Researchers with SDSC's Cooperative Association for Internet Data Analysis (CAIDA) *Trestles* to perform simulations of the universe's growing causal network. By parallelizing and optimizing the application, Robert Sinkovits, a computational scientist with SDSC, was able to complete in just over one day a computation that was originally projected to require three to four years.
Please see http://www.sdsc.edu/News%20Items/PR111912_network_cosmology.html for the full press release.

SDSC Wins HPCwire Editors' Choice Awards for 'Data Oasis' Storage System

SDSC was recognized by HPCwire, a top online publication covering high-performance computing and related technologies, for the Center's innovative *Data Oasis* parallel file storage system. SDSC was presented with 'Editor's Choice: Best HPC Storage Product or Technology, for the *Data Oasis* Storage File System on *Gordon*' as part of the publication's annual awards announced at SC12 in Salt Lake City, Utah, in November.
SDSC earlier this year completed deployment of its Lustre-based *Data Oasis* parallel file system, with has four petabytes (PB) of capacity and 100 gigabytes per second (GB/s) to handle the data-intensive needs of the center's new *Gordon* supercomputer, in addition to its *Trestles* and *Triton* compute clusters. For the full press release please see http://www.sdsc.edu/News%20Items/PR111412_hpcwire_award.html.

19.3 User-facing Activities

19.3.1 System Activities

Notable systems activities during the last quarter included:

- Replacement of all the RAID cards in Data Oasis
- Preparing for the NSF project storage expansion
- Supporting dedicated project Gordon I/O nodes

The most significant systems work this quarter was the replacement of all 128 RAID cards in the Data Oasis file servers in October. The Data Oasis hardware vendor, Aeon Computing (via subcontract from Appro), identified an incorrectly specified resistor on the cards. Under certain loads, the resistor would overheat and trigger a reset of the card and intermittent loss of access to the card's drives. After reproducing the problem, Aeon Computing received updated cards from LSI, the component vendor. The replacement work was done in two stages: first, we upgraded the cards in the 16 servers supporting the UCSD resource Triton; after a week of testing an observation, we replaced the cards in the 48 servers providing storage for the Trestles and Gordon Lustre scratch and NSF project space. In both cases the work was completed in less than a day with no loss of data. Where possible, gateway users (e.g., CIPRES) were able to continue running through the maintenance window. This was a no-cost fix to the project.

In addition to preventative and routine maintenance on Data Oasis, we have begun preparation for the added storage as part of Gordon, which will be incorporated into the Lustre file system used for NSF project storage. The expansion will involve upgrading the current drives from 2TB to 3TB, and adding JBODs to the 8 existing storage servers (this design was chosen in part to maintain the current per-server performance). Other preparation efforts included reviewing the current allocations and usage of the project space, and following up with PIs when necessary to reduce usage or request additional storage. This is to ensure that we can align file system quotas and allocation after the upgrade. Hardware testing and validation of the new storage design is in process, and the expansion should be completed during the first quarter of 2013. In parallel, SDSC is participating in XSEDE activities that are leading to the having storage become part of the standard XSEDE allocations process.

The dedicated Gordon I/O nodes continue to be specialized resources, requiring customization for each project. Beyond the applications, each project has its own storage, firewall, and access configuration needs. As each project comes along we try to provide controlled access to systems level activities, such as restarting services, where appropriate. Over time, we hope to minimize the work required by the systems team, while still maintaining the stability and integrity of Gordon as a whole. We consider the work on these I/O node projects one of the unique capabilities that Gordon offers to the data-intensive community, some of which are discussed in the "SP Collaborations" section below.

There were a couple of brief hardware outages with wide impact. The first was the loss of the routing engine in the router handling SDSC's connection to the XSEDE network. This led to repeated losses of connectivity on the public interfaces of Gordon during the few days while a replacement part was shipped. The second event occurred in late December, and was due to a bug in the Linux kernel used on Gordon that resulted in a kernel panic on nodes that had been up for approximately 210 days. While the Gordon compute nodes undergo periodic reboots for software updates or to clear hung tasks, the I/O nodes acting as Lustre routers do not, and a reboot of the impacted I/O nodes was required.

19.3.2 Services Activities

Between the two tickets systems used to support Trestles and Gordon (the XSEDE ticket system and SDSC's local ticket system) a total of 368 tickets were created between October 1 and December 31, 2012. These tickets included account questions, file system issues, software requests, Globus support, code support, password resets, code optimizations and debugging, allocation refunds/problems, project space requests, software support, licensing queries, and resource availability. 303 of those tickets were closed, leaving 65 tickets that we are still working to resolve. The average time to close the tickets across the two systems was 8 days, with a median time of 3 days.

Gordon is now in its fourth quarter of operation and supporting users from 4 XRAC allocation cycles. Typical *Gordon* support included fielding questions and providing information on Gordon's architecture, software install requests, utilizing SSD scratch space, and performance analysis for jobs spanning multiple switches, and utilizing vSMP nodes. The Hadoop installation on Gordon was put into production in the past quarter. Additional software installs include new versions of the PGI compilers, R modules, Abaqus and VisIt software.

In support of *Trestles* users, SDSC user services staff fielded questions on gridftp usage, allocations/accounts, new software installs, system performance, software licensing, filesystem use/troubleshooting, and projects space requests. New software installs/support included dppdiv (v 1.0b), namd, tophat (v.2.0.6), Amber, mesa, desmond, Abaqus, and VisIt. Additionally, SDSC user services staff recompiled and improved the performance of the VASP install on Trestles. Fixes to CTSS components were made to resolve problems with RDR Trestles decommission display and with proper upload of Job and Load information to XSEDE central information services. We worked with the GRIDCHEM gateway team on an issue related to job submission to Trestles.

19.4 Security

SDSC saw no new security incidents this quarter on *Gordon* nor *Trestles*.

During this quarter, we completed the security assessment of the *Trestles* upgrade and incorporated the additional controls, configuration, and customized programs in a *Rocks Roll* for rapid, convenient deployment. In addition, we have started to design and implement new controls and procedures to support projects on dedicated *Gordon* resources that would otherwise conflict with *Gordon's* existing security controls and policies.

19.5 Education, Outreach, and Training Activities

EOT activities are summarized in the table below.

Type	Audiences	Title	Location	Date(s)	Hrs	# Participants	# Under-rep.	Method
		TRAINING						
Tutorial	F. D. G. U. I.	Intro to Scientific Visualization and Remote Visualization on Gordon (Chourasia)	UCSD/SDSC	October 24	4	89	9	Sync, web
Tutorial	F. D. G. U. I.	Introduction to Predictive Analytics for Big Data (Balac)	UCSD/SDSC	December 11	2	102	18	Sync, web
Workshop	F. D. G. I.	PACE: Data Mining Boot Camp 1 (Balac)	UCSD/SDSC	October 16-17	16	35	10	Sync
		EDUCATION						
Workshop	S	Girl Scout Event: Alice: Beginning Programming in a 3D Environment	SDSC	October 13, 2012	6	22	22	Sync
Workshop	S	SMART Team 1st Qualification Phase Meeting	TSRI	October 13, 2012	3	39	17	Sync
Workshop	S	SMART Team JMol Class w/ David Goodsell	SDSC	October 20, 2012	3	19	8	Sync
Workshop	S	Alice: Beginning Programming in a 3D Environment	SDSC	October 27, 2012	6	22	4	Sync
Workshop	T	TeacherTECH Alice Workshop – Five Part Series	SDSC	November 7, 2012	2	17	12	Sync
Workshop	S	SDSC Triton Quiz Bowl	SDSC	November 10, 2012	8	140	70	Sync
Workshop	T	CSTA/SDSC Education Partnership Meeting	SDSC	November 13, 2012	2	19	6	Sync
Workshop	T	TeacherTECH Alice Workshop – Five Part Series	SDSC	November 14, 2012	2	17	12	Sync
Workshop	T	TeacherTECH Alice Workshop – Five Part Series	SDSC	November 28, 2012	2	17	12	Sync
Workshop	S	Alice: Beginning Programming in a	SDSC	December 1, 2012	6	20	20	Sync

		3D Environment (BE WISE)						
Work shop	T	TeacherTECH Alice Workshop – Five Part Series	SDSC	December 5, 2012	2	17	12	Sync
Work shop	S	SMART Team Mentor Match and Lab Tours	TSRI	December 6, 2012	3	36	12	Sync
		OUTREACH						
Conf	F. D. G. U. I.	Super Computing 2012 *(SC12): Individual topics and presenters below*	Salt Lake City, UT	**November** 9-15	30	10,000	1000	Sync
Conf	F. D. G. U. I.	*GORDON: How Flash Accelerates Data-Intensive Computing* (Norman)	Salt Lake City, UT	13				Sync
Conf	F. D. G. U. I.	*SDSC's GORDON Q&A* (Strande et al)	Salt Lake City, UT	13				Sync
Conf	F. D. G. U. I.	***DATA OASIS****: SDSC's High-Performance Parallel File System* (Moore et al)	Salt Lake City, UT	13				Sync
Conf	F. D. G. U. I.	***SDSC's TRESTLES****: High-Productivity Workhorse (*Moore)	Salt Lake City, UT	13				Sync
Conf	F. D. G. U. I.	*SDSC's Cloud Infrastructure for Scientific Research* (Hawkins)	Salt Lake City, UT	13				Sync
Conf	F. D. G. U. I.	*Flash Technology in High-Performance Computing Accelerates scientific Discovery* (Cicotti)	Salt Lake City, UT	13				Sync
Conf	F. D. G. U. I.	*Data-Intensive Computing at SDSC* (Norman)	Salt Lake City, UT	13				Sync
Conf	F. D. G. U. I.	*Successes with Large Memory vSMP Applications on SDSC's Gordon System* (Sinkovits)	Salt Lake City, UT	14				Sync
Conf	F. D. G. U. I.	*Neuroscience Gateway* (Majumdar)	Salt Lake City, UT	14				Sync

Conf	F. D. G. U. I.	*Data Analytics at SDSC* (Wolter)	Salt Lake City, UT	14				Sync
Conf	F. D. G. U. I.	*Big Data Benchmarking* (Baru)	Salt Lake City, UT	14				Sync
Conf	F. D. G. U. I.	*Enabling Phylogenetic Research via the CiPRES Science Gateway* (Pfeiffer)	Salt Lake City, UT	14				Sync
Conf	F. D. G. U. I.	***GORDON**: Design and Performance of a 3D Torus Interconnect for Data-Intensive Computing (*Strande)	Salt Lake City, UT	14				Sync
Conf	F. D. G. U. I.	*Non-traditional Users* (Sinkovits)	Salt Lake City, UT	14				Sync
Conf	F. D. G. U. I.	*Meet-N-Greet XSEDE Users* (Strande)	Salt Lake City, UT	14				Sync
Conf	F. D. G. U. I.	*Finding Somatic Mutations in the Genomes of a 115-Year-Old Woman* (Pfeiffer)	Salt Lake City, UT	14				Sync
Conf	F. D. G. U. I.	*Mapreduce Clustering of Large Datasets of Protein-Ligand Binding Geometries on Gordon* (Taufer)	Salt Lake City, UT	14				Sync
Conf	F. D. G. U. I.	*HADOOP on SDSC's Gordon Data-Intensive Cluster* (Tateneni)	Salt Lake City, UT	14				Sync
Conf	F. D. G. U. I.	SDSC Data Infrastructure Overview (Norman)	Salt Lake City, UT	14				Sync

* *S=synchronous, A=asynchronous*

19.6 Training

The fourth quarter of 2012 training reflected growing community interest in SDSC's newest XSEDE resources. SDSC led two short tutorials and one two-day workshop around predictive data analytics and data visualization, reaching nearly 200 participants on-site and via webcast. The half day workshop on visualization (simultaneously conducted in-person and online) drew more than 100 participants from 55 organizations and over 30 disciplines.

19.6.1 *Education*

A series of "Introduction to Computer Science Principles through Alice" workshops for students (StudentTECH) and teachers (TeacherTECH) served both short-term and long-term goals. Student versions attracted diverse audiences, many with full scholarships, seeking to increase early engagement and strengthen recruitment into more advanced CS courses and computational sciences, as well as stimulate regional science fair projects in both areas (XSEDE-xy student poster competition participants are often recruited through the regional science fairs). TeacherTECH "Alice" workshops both introduced participants to Alice as a way to teach CS principles, and recruited 2013 participants for the SDSC CE21 project in the region.

Planning took place for an extended "CS Principles through Alice" workshop series to be offered after school on a local charter school site in southeast San Diego. This series will attract students from the school itself as well as the local area, both of which are predominantly underrepresented in computing. At the same time, teachers from that school will join the course as apprentices, to add to their own professional development.

Impacts: Two teachers from the TeacherTECH Alice workshop series will assist with the APCHS after-school classes. The sixteen participating teachers are candidates for SDSC's April 2013 Computer Science Principles and Pedagogy professional training. From this group will be recruited the Year 2 cohort for the San Diego regional CE21 project.

Students from the introductory Alice workshops are building demand for more advanced programs, leading to current planning for student parallel programming, data visualization, and Java programming workshops for spring and summer 2013.

19.6.2 *Outreach*

XSEDE TEOS Blog: SDSC's Ange Mason posted 49 articles to the XSEDE TEOS blog in the past quarter through a combination of single news posts and the XSEDE weekly HPC Research and Education newsletter posts. This brings the 2012 total to 184 posts.

SDSC's Ange Mason continued updating and managing the HPC University website with content including news, events, career postings, and internship and fellowship opportunities. The HPCU site continues to grow toward becoming a resource and information-rich site.

To expand the audience, a new (in progress) online resource "Computational Science Education News" Facebook page will feature a combination of content from the XSEDE blog and HPCU.

SDSC Outreach activities for October through December focused on students, teachers, and researchers. SMART Teams collaborations for 2012-13 launched with Steve Connelly of The Scripps Research Institute in La Jolla. Revisions from the 2011-2012 year seek to maximize the educational and mentoring value of each student/research meeting.

SDSC staff extended outreach to national and international colleagues through professional conference presentations and tutorials related to XSEDE Data-Intensive computational services are included in the table above. SDSC had a major presence at Supercomputing 12, with nineteen presentations related to XSEDE, Gordon, and Data-Intensive Computational Science Discovery.

19.7 SP Collaborations

19.7.1 *Collaborations with SP XSEDE Users*

- Pietro Cicotti initiated collaboration with Lorne Leonard (PSU) to evaluate and improve the scalability of the PIHM (Penn State Integrated Hydrologic Modeling System). This work could potentially lead to better modeling of significant hydrologic events.

- Mahidhar Tatineni and Pietro Cicotti worked with Yoav Freud (UCSD) to deploy and configure a dedicated Hadoop cluster for a large data analytics class. This Hadoop instance was built from a Gordon I/O node and 16 compute nodes. Freund has an education allocation on Gordon.
- Pietro Cicotti completed collaboration with the Protein Data Bank (PDB) to determine the impact of using Gordon's flash drives for a large-scale structural alignment project. Speedups of 3.8x and 5.8x were achieved using Gordon's existing Lyndonville flash drives and an early release of Intel's new Taylorsville flash drives, respectively, relative to the PDB's current hard disk based system which leverage OSG.
- Amit Chourasia provided visualization support for the following projects
    - Visualization of ENZO simulations on Gordon (Mike Norman, UCSD): Together with Hank Childs (LBL), initiated discussions on how to utilize Gordon's unique architecture to speedup and interleave visualization with the computations.
    - Visualization of GigaLES simulation data (John Helly, SIO/UCSD)
- Amit Chourasia worked closely with Darcy Ogden (SIO/UCSD) to improve the performance and scalability of CFDLib and continued work on visualization of volcanic jets. Together they extracted and analyzed more detailed, quantitative results from the simulations. The main goal of this work is to understand the tightly coupled interaction between jet dynamics and crater growth. This suite of visualization efforts focused on quantifying each of these processes. Specific work conducted during past quarter and applied to all nine simulation data sets include
    - Visualizing cross sections at various depths for six different temporal variables
    - Computation of plume area at a given cross section depth
    - Plots of crater growth profiles
    - Topography of plume boundary at last time step
- Dongju Choi led ECSS collaboration with David Hausser's team (UCSC) to efficiently run the whole genome alignment pipeline at SDSC. To date we were able to port the JobTree software to Gordon and integrate with the Torque scheduler. We also resolved questions related to the Python version, memory requirements on the Tokyo Tycoon servers and scheduler wait time issues. The worker aligner now has basic functionality on Gordon using JobTree and Tokyo Tycoon and we have started further tuning of the aligner. The team is now ready to start longer test runs in the 2nd quarter of this project.
- Robert Sinkovits continued his collaboration with Mao Ye (U. Illinois) to improve performance and usability of limit order book application, which is used to evaluate the impact of high frequency trading on markets.
- Robert Sinkovits, working with Doug White (UC Irvine), evaluated and ported clique detection algorithms to Gordon and developed scripts for post-processing results. These algorithms play a key role in White's social science research on identifying maximally cohesive groups.
- Amit Majumdar, Subhashini Sivagnanam & Kenneth Yoshimoto, collaborating with Ted Carnevale & Michael Hines from Yale School of Medicine and MaryAnn Martone, Anita Bandrowski & Vadmin Astakhov from NIF, continued development of the Neuroscience Gateway. A poster presentation and a booth demonstration were done at the Society for Neurosciences meeting in New Orleans in October 2012. Accounts have been created for early users who have been using the Neuroscience Gateway (NSG Portal). The users have been running models using NEURON software on Trestles.
- Paul Rodriguez continued to work with James Fowler (UCSD) to efficiently run R simulations in parallel on Gordon in support of Fowler's political science research.
- Wayne Pfeiffer made expedited runs of various phylogenetics codes for CIPRES gateway

users whose original attempts exceeded wall clock limits, were projected to exceed time limits or simply failed. A summary of these runs is given below

- BEAST 1.7.3 on Trestles for
  - Vicky Pritchard, formerly of UC Santa Cruz and the National Marine Fisheries Service (336 hours)
- BEAST 1.7.4 on Gordon to take advantage of faster run times for
  - Pierre-Henri Fabre of the University of Copenhagen (202 hours, 178 hours, and 246 hours)
  - Rachel Life of the University of Washington and the Western Fisheries Research Center (302 hours)
- MrBayes 3.2.1 on Gordon for
  - Giovanni Zecca of the University of Milan (253 hours)
  - Zhouying Xu, formerly of Cornell University and currently at the Northwest Sci-Tech University of Agriculture and Forestry in China (188 hours)
  - Mare Nazaire of Washington State University (9 hours)
  - Jerry Cooper of Landcare Research in New Zealand (10 hours).

Zecca, Xu and Nazaire had previously submitted jobs that failed to converge within a week using the old, 3.1.2h version of MrBayes on Gordon. With the new version of the code, Nazaire's job converged dramatically faster. Zecca's and Xu's jobs achieved better convergence values, but eventually stopped converging, presumably because of limitations in their data. Cooper's original job failed because of an apparent bug in the old version of MrBayes, but worked fine with the new version.

19.7.2 Collaborations with External Partners

Rick Wagner and Steve Meier have been working with Dmitry Mishin from Johns Hopkins University on the deployment of VOBox, a Dropbox-like tool for the digital astronomy, using SDSC Cloud as the backend storage layer. In addition to object storage capabilities, VOBox also provides a flexible means for custom metadata extraction that can be used to drive data search and retrieval services.

Amit Chourasia initiated a new collaboration on visualization of ENZO on Gordon with Hank Childs & David Camp at LBL and Michael Norman, Robert Harkness, Geoffrey So, Rick Wagner.

19.8 SP-Specific Activities

Scheduling and Resource Optimization

SDSC again surpassed its availability goals for the XCDB (XSEDE central database) and the AMIE central instance in Q4. There were only 5 minutes of downtime and that was during a planned maintenance window. We also failed over the database to its backup site at PSC and failed it back without incident to avoid a service outage during network maintenance at SDSC. In 2013 we plan to upgrade Postgresql to take advantage of new features and because support for the current version expires in 2014.

Performance tuning was done for topology scheduling in Catalina Scheduler for the Gordon machine. This was coded, but not yet installed into production. To accommodate long-running jobs on the Gordon vSMP nodes for CIPRES gateway, queue wallclock limits were increased.

Software

A test instance of Unicore was installed for test at SDSC. This was part of Basic EMS Acceptance Test Activity 97.

Miscellaneous XSEDE Activities

SDSC continues to be very active in XSEDE through various working groups and the Service Provider Forum. These included:

- Development and deployment of storage allocations
- XWFS pilot project
- XRAC reviews
- Allocations-related policy and process issues

19.9 Publications

Grand, S.; Goetz, A.W.; Walker, R.C., "**SPFP: Speed without compromise - a mixed precision model for GPU accelerated molecular dynamics simulations.**", Computer Physics Communication, **2012**3 184, pp374-280. DOI: 10.1016/j.cpc.2012.09.022

Park, K.; Goetz, A.W.; Walker, R.C.; Paesani, F., "**Adaptive QM/MM molecular dynamics simulations of aqueous systems.**", Journal of Chemical Theory and Computation, **2012**, 8 (8), pp 2868–2877, DOI: 10.1021/ct300331f

M. Tatineni, A. Majumdar, "Optimizing Hadoop Deployment on Gordon Data Intensive Supercomputer," Second Workshop on Big Data Benchmarking, Dec. 17-18, Pune, India, 2012.

N.T. Carnevale, S. Sivagnanam, K. K. Yoshimoto, V. Astakhov, A. E. Bandrowski, M. E. Martone, A. Majumdar, "A Neuroscience Gateway for High Performance Computing," Society for Neuroscience Annual Meeting, New Orleans, October 13-17, 2012.

SDSC, Intel, "Flash Technology in High-Performance Computing Accelerates Scientific Discovery". Intel white paper. November 2012. Available at: http://www.intel.com/content/www/us/en/solid-state-drives/ssd-dc-s3700-sdsc-study.html

19.10 Metrics

Appendices 1.9A-C includes the following metrics:

- 1.9-A XSEDE-generated user ticket statistics
- 1.9-B *Trestles* and *Gordon* Quarterly stats from XDMoD (July – September 2012)
- 1.9-C Local *Trestles* stats related to achieving user productivity objectives

Appendix 1.9A Standard User Assistance Metrics

Time to Resolution	account issues	file systems	grid software	jobs/batch queues	login/access issues	mss/data issues	network issues	software/apps	system issues	other
0-1 hr		1			2					1
1-24 hr	2	5		16	4	1		14	4	5
1-7 d	5	12	1	33	8	7		6	4	4
1-2 wk	2	4		14	1	1		4		1
> 2 wk	4	3	1	33	8	4	1	20		6
Still Open	2	1	2	29	2	2		14	1	3

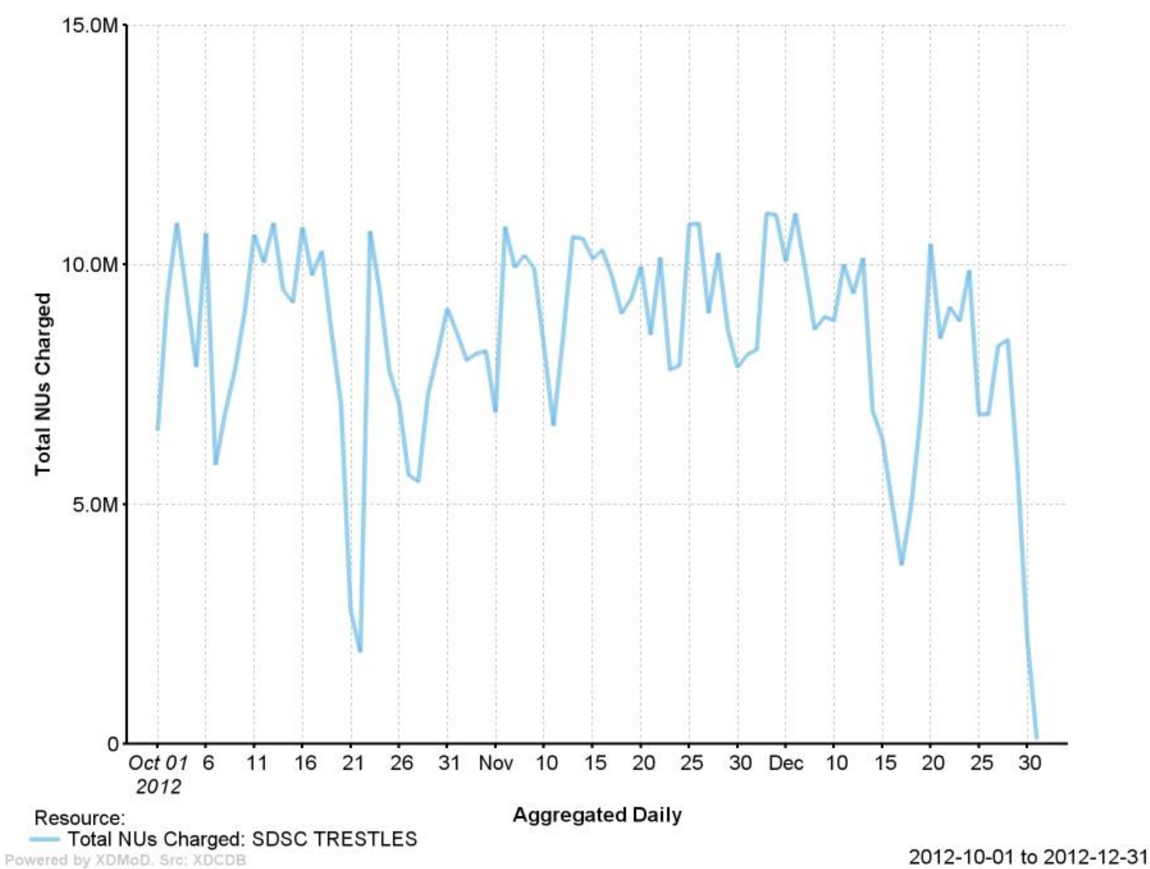
Appendix 1.9B Trestles and Gordon Quarterly Usage Statistics

SDSC-TRESTLES Quarterly Report

Total NUs Charged by Resource

Service Provider = SDSC

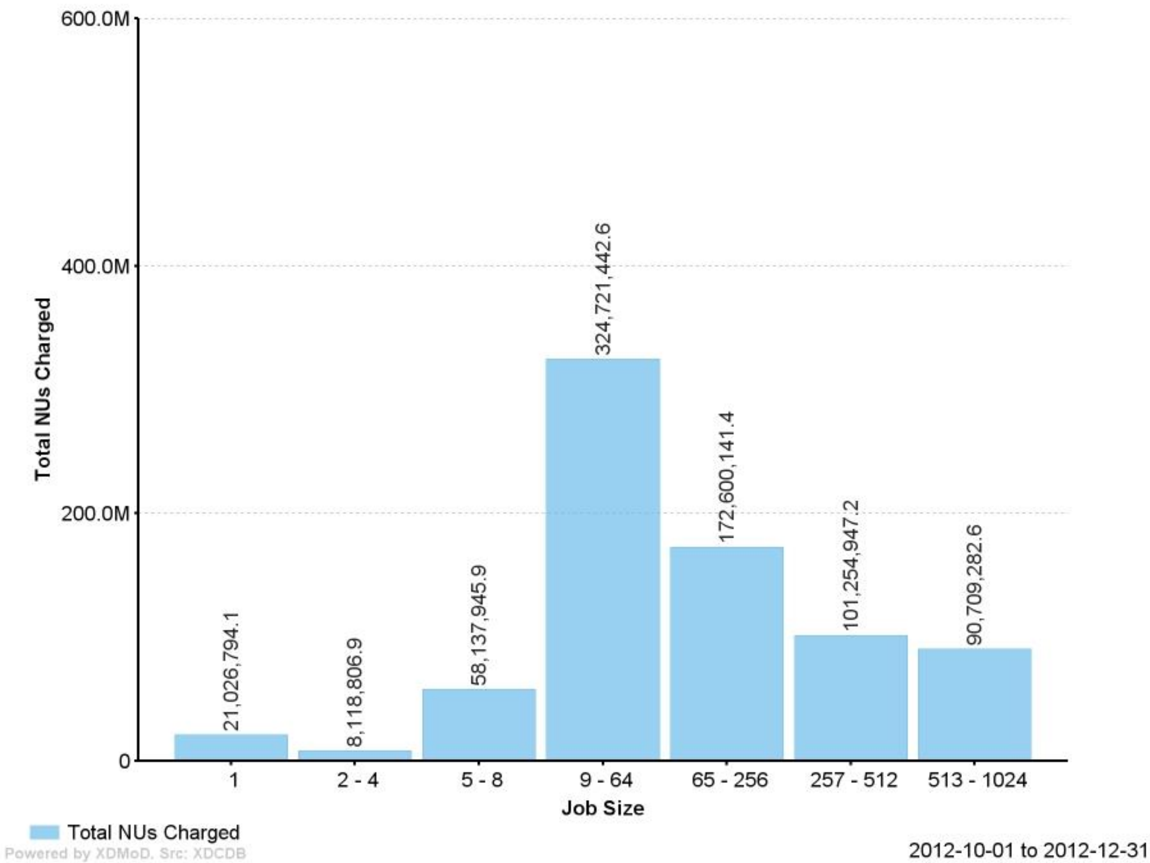
2012-10-01 to 2012-12-31



Total NUs Charged by Job Size

Resource = SDSC-TRESTLES

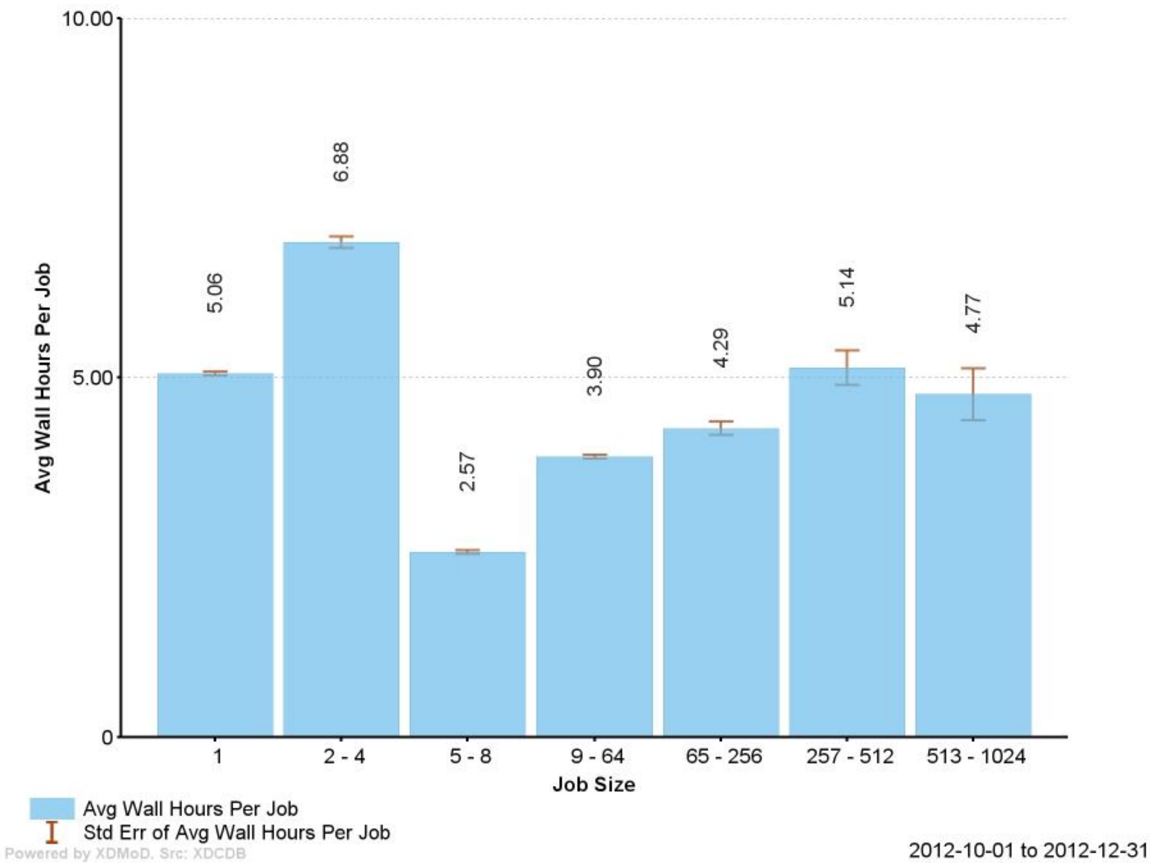
2012-10-01 to 2012-12-31



Avg Wall Hours Per Job by Job Size

Resource = SDSC-TRESTLES

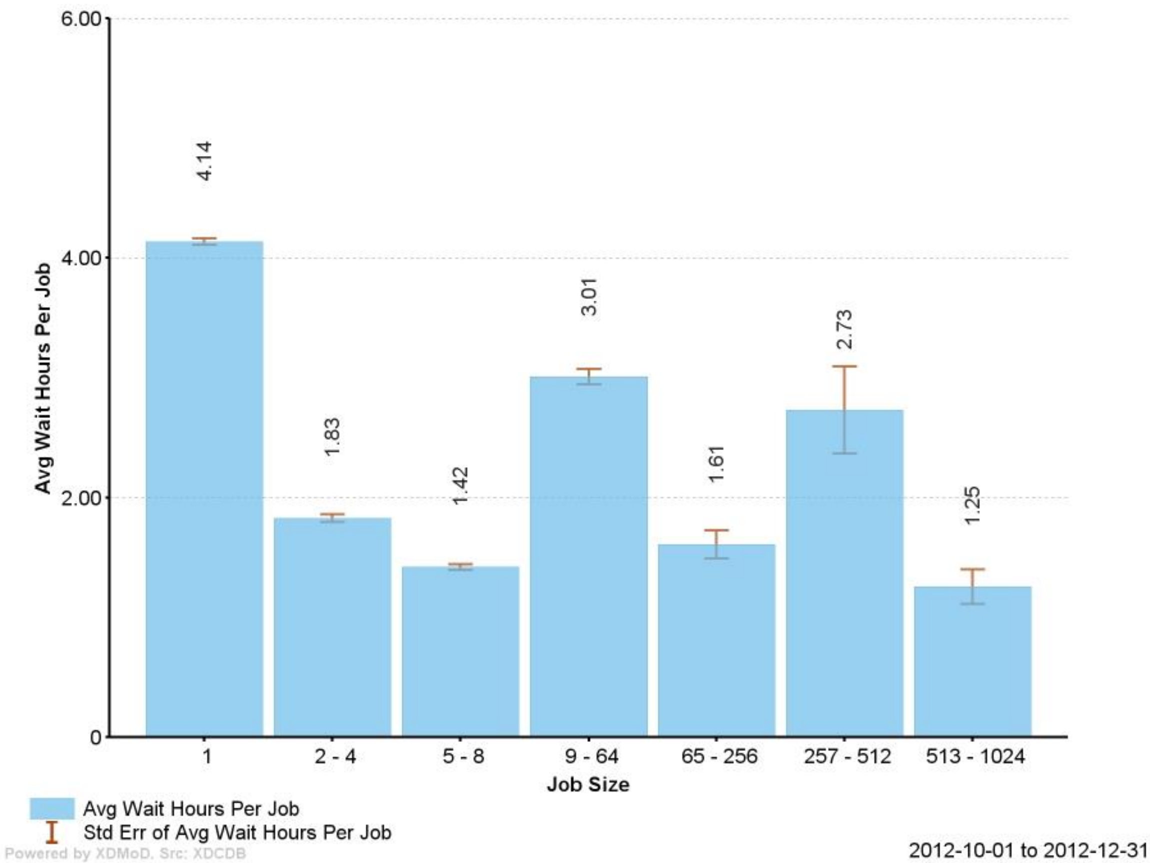
2012-10-01 to 2012-12-31



Avg Wait Hours Per Job by Job Size

Resource = SDSC-TRESTLES

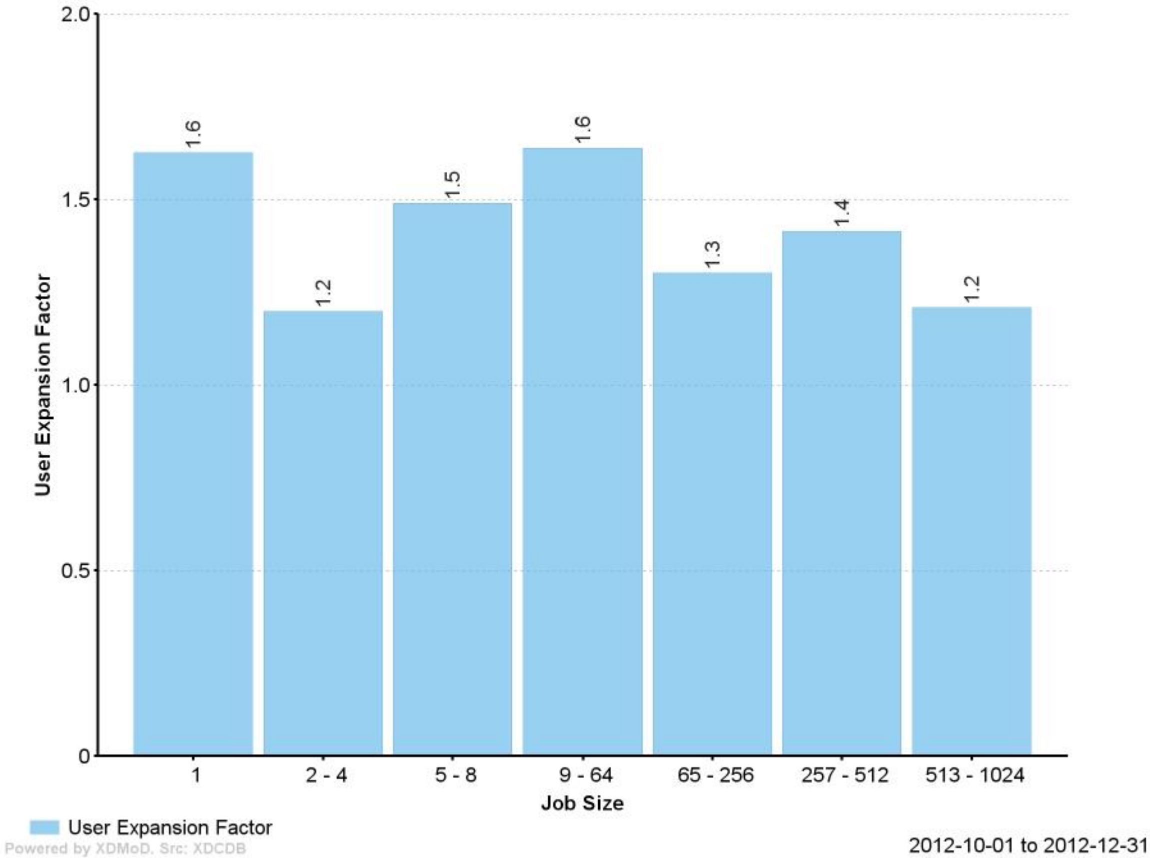
2012-10-01 to 2012-12-31



User Expansion Factor by Job Size

Resource = SDSC-TRESTLES

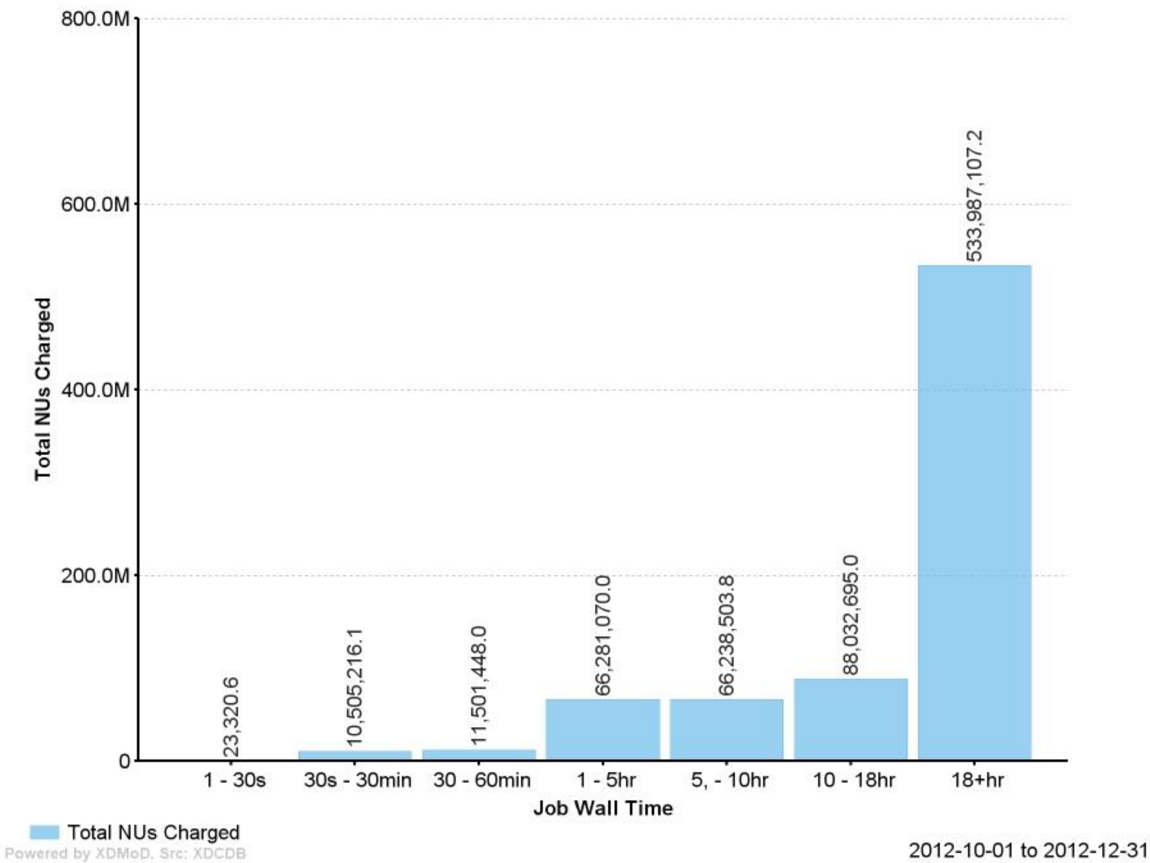
2012-10-01 to 2012-12-31



Total NUs Charged by Job Wall Time

Resource = SDSC-TRESTLES

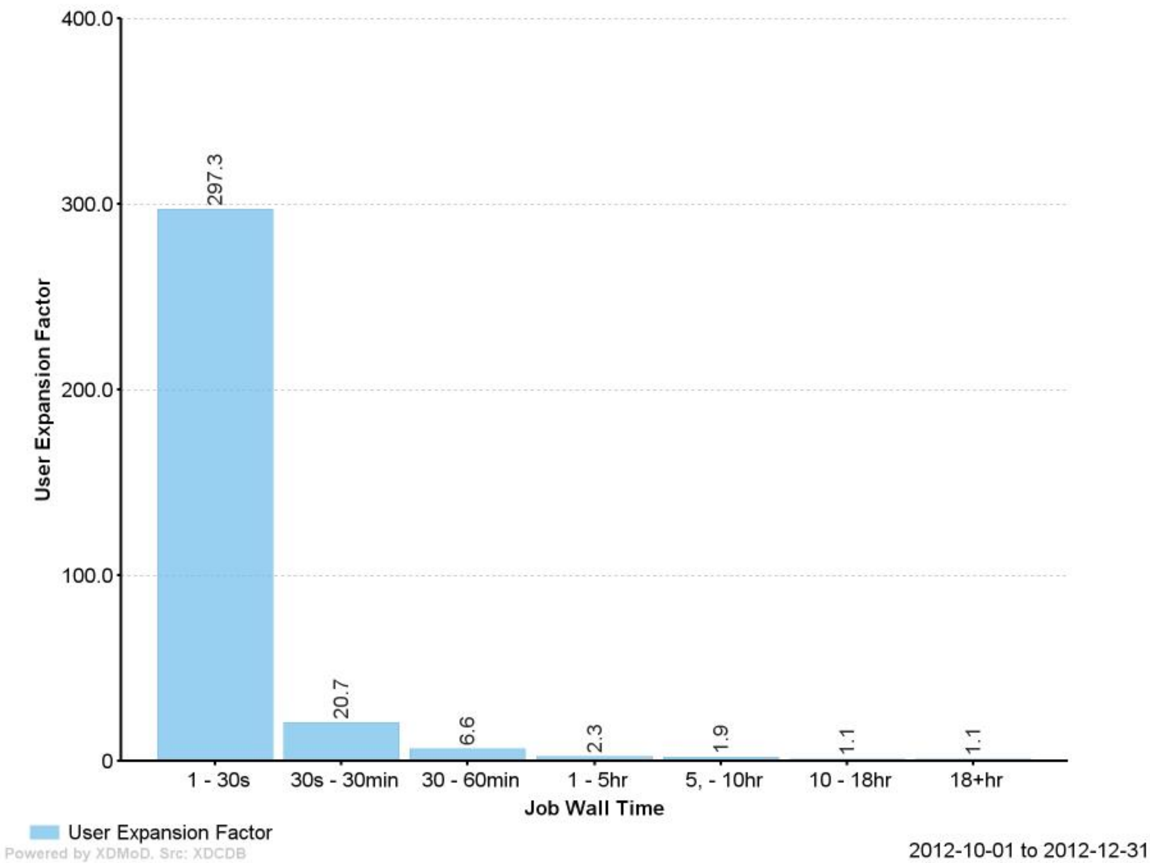
2012-10-01 to 2012-12-31



User Expansion Factor by Job Wall Time

Resource = SDSC-TRESTLES -- Service Provider = SDSC

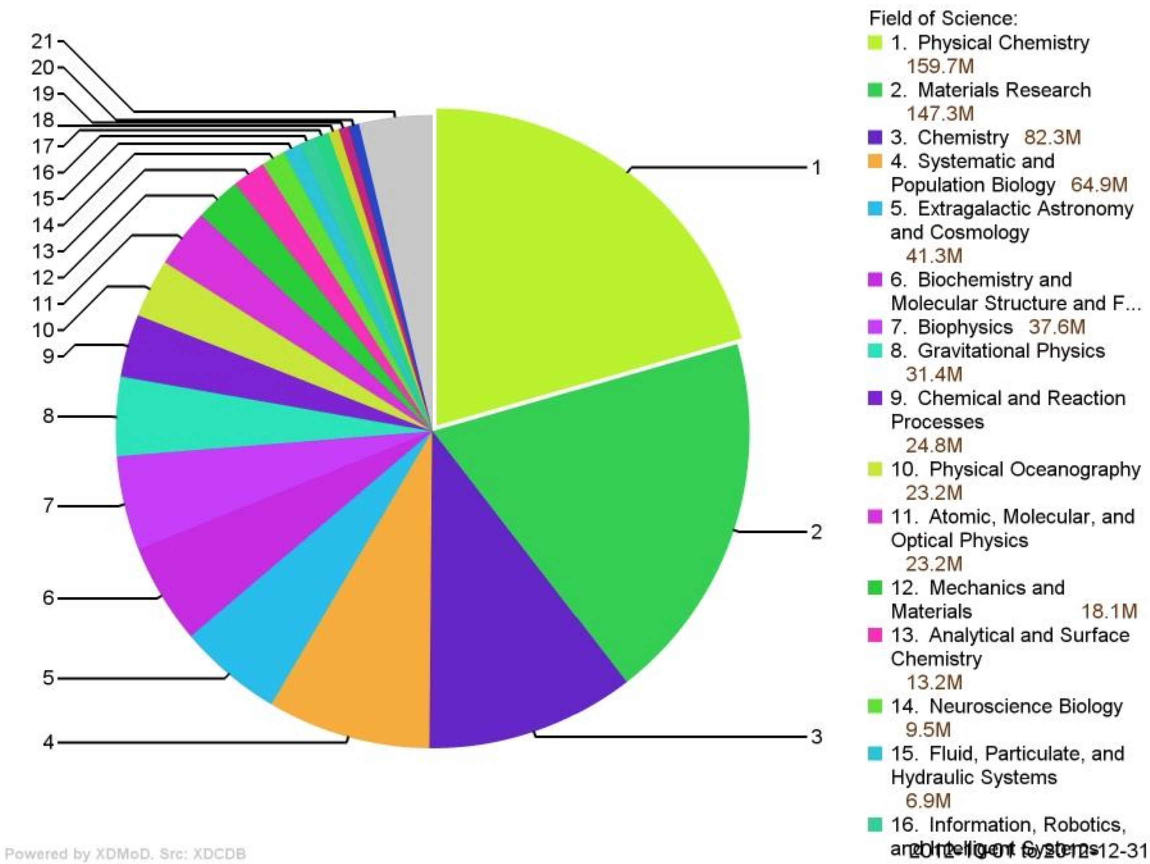
2012-10-01 to 2012-12-31



Total NUs Charged by Field of Science

Resource = SDSC-TRESTLES

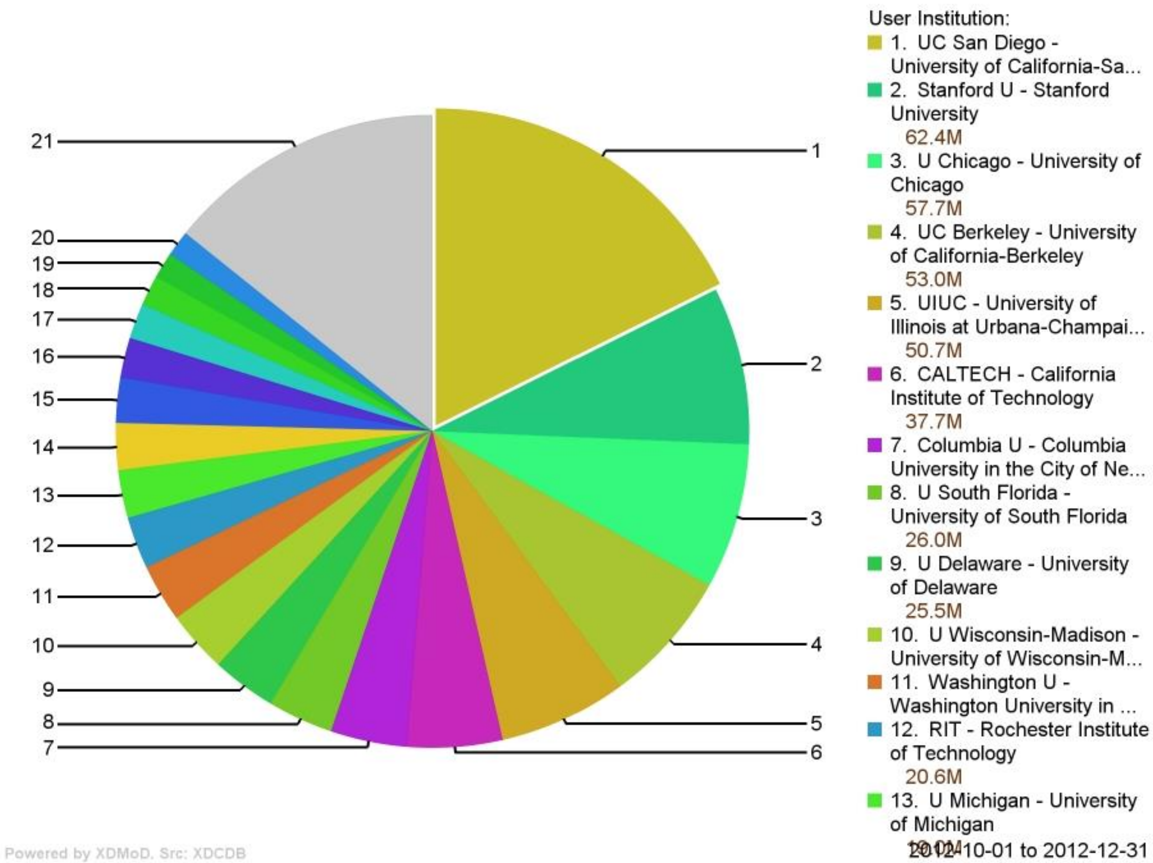
2012-10-01 to 2012-12-31



Total NUs Charged by User Institution

Resource = SDSC-TRESTLES

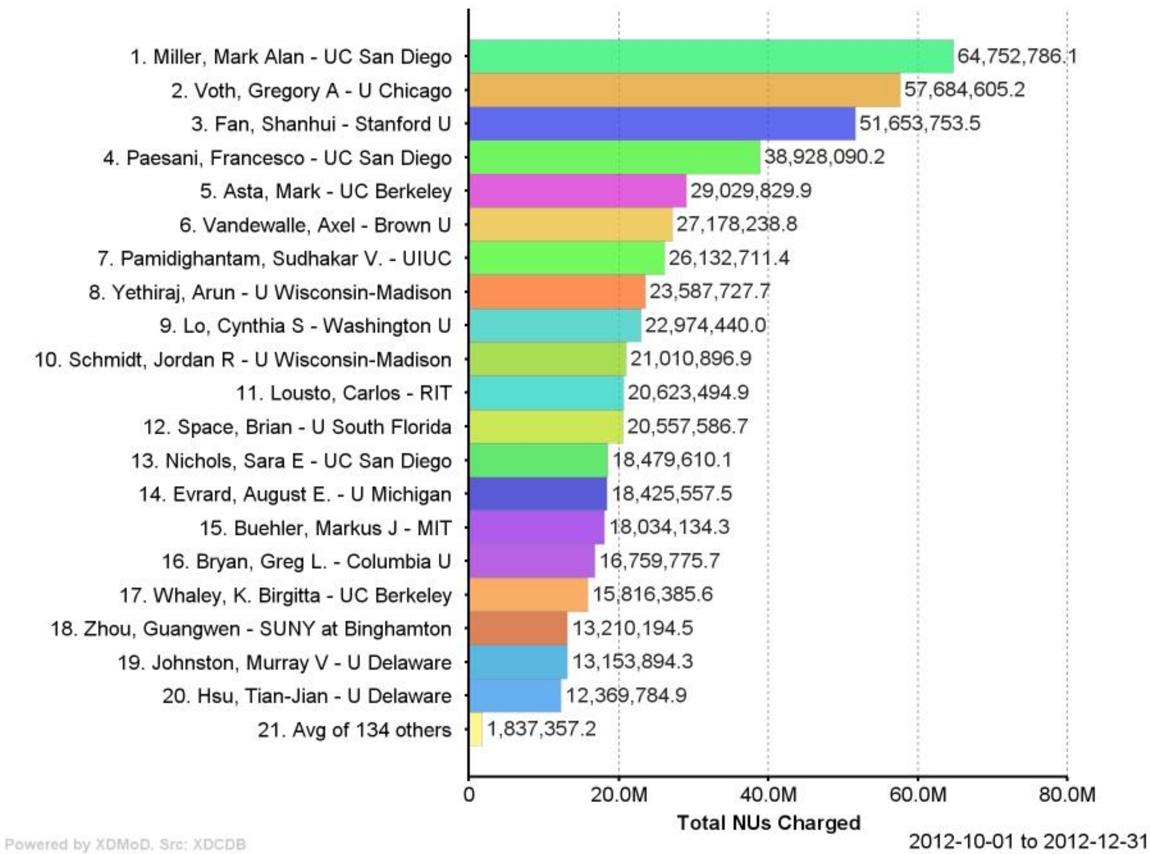
2012-10-01 to 2012-12-31



Total NUs Charged by PI

Resource = SDSC-TRESTLES

2012-10-01 to 2012-12-31

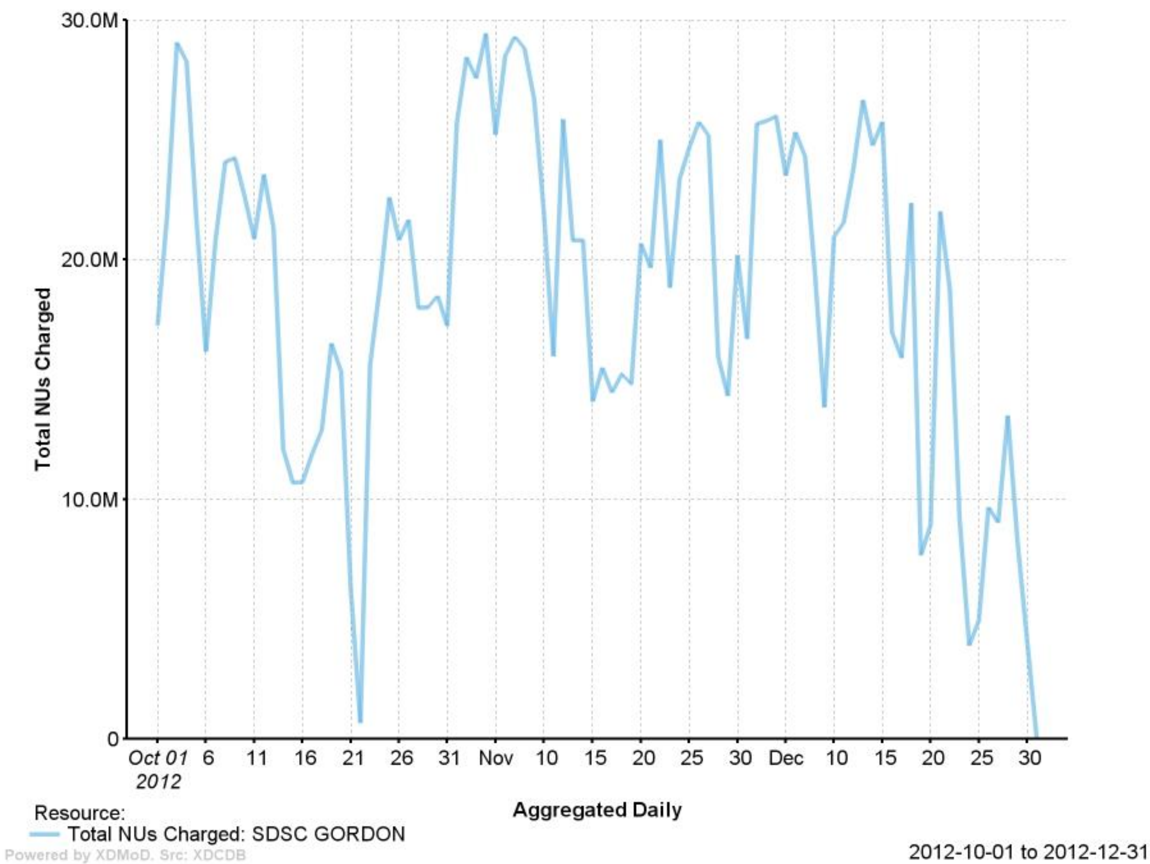


SDSC-GORDON Quarterly Report

Total NUs Charged by Resource

Service Provider = SDSC

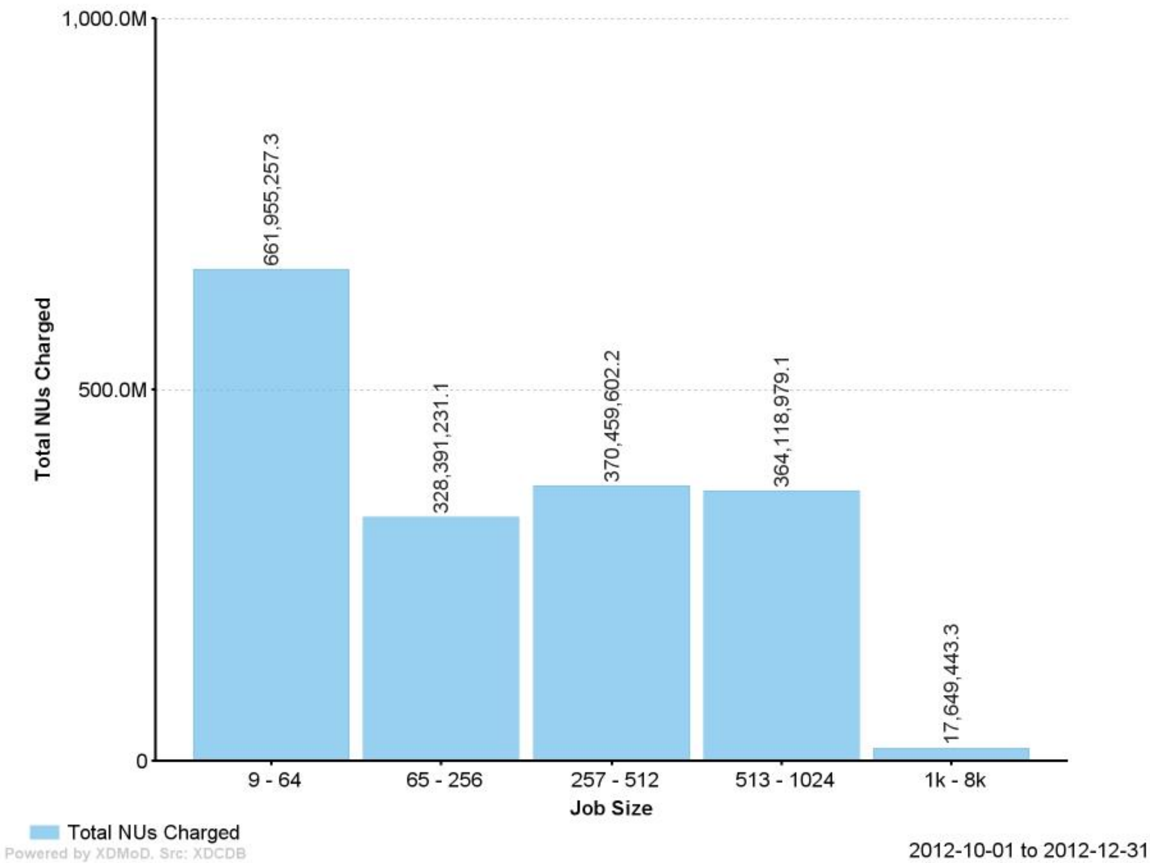
2012-10-01 to 2012-12-31



Total NUs Charged by Job Size

Resource = SDSC-GORDON

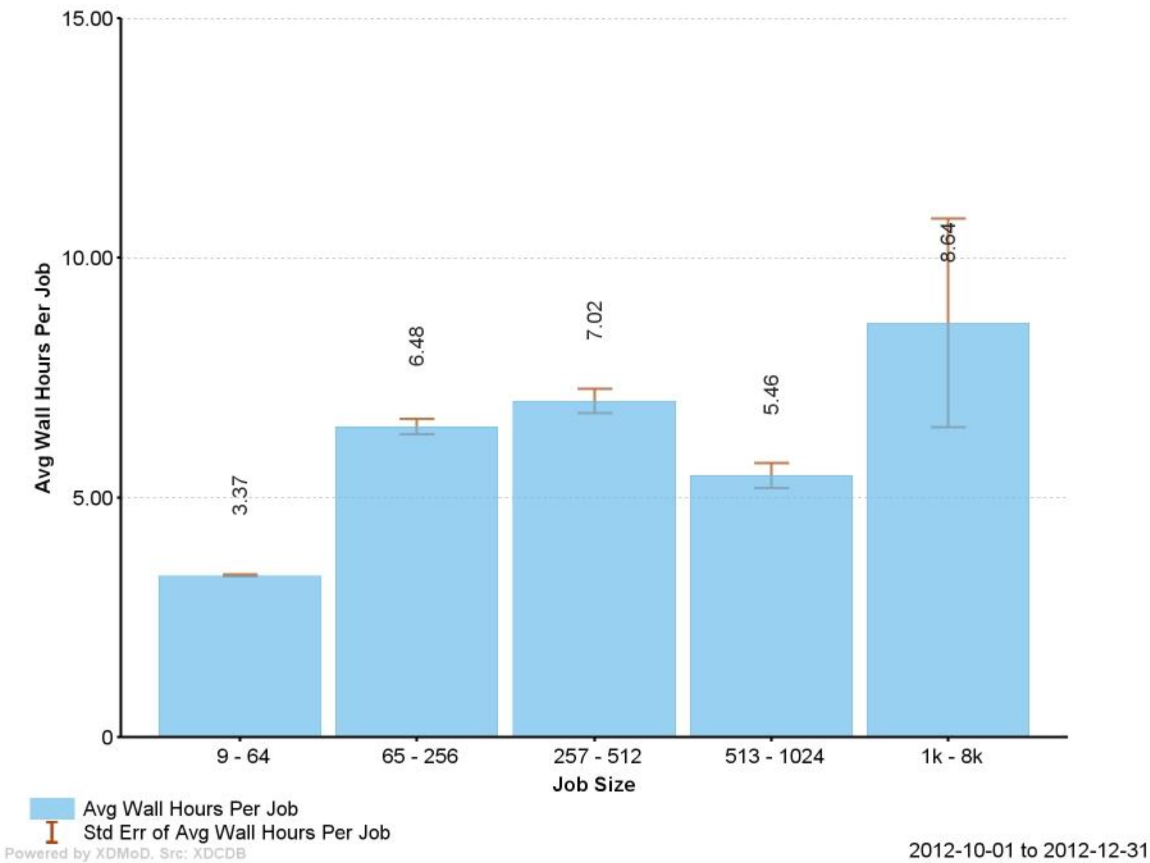
2012-10-01 to 2012-12-31



Avg Wall Hours Per Job by Job Size

Resource = SDSC-GORDON

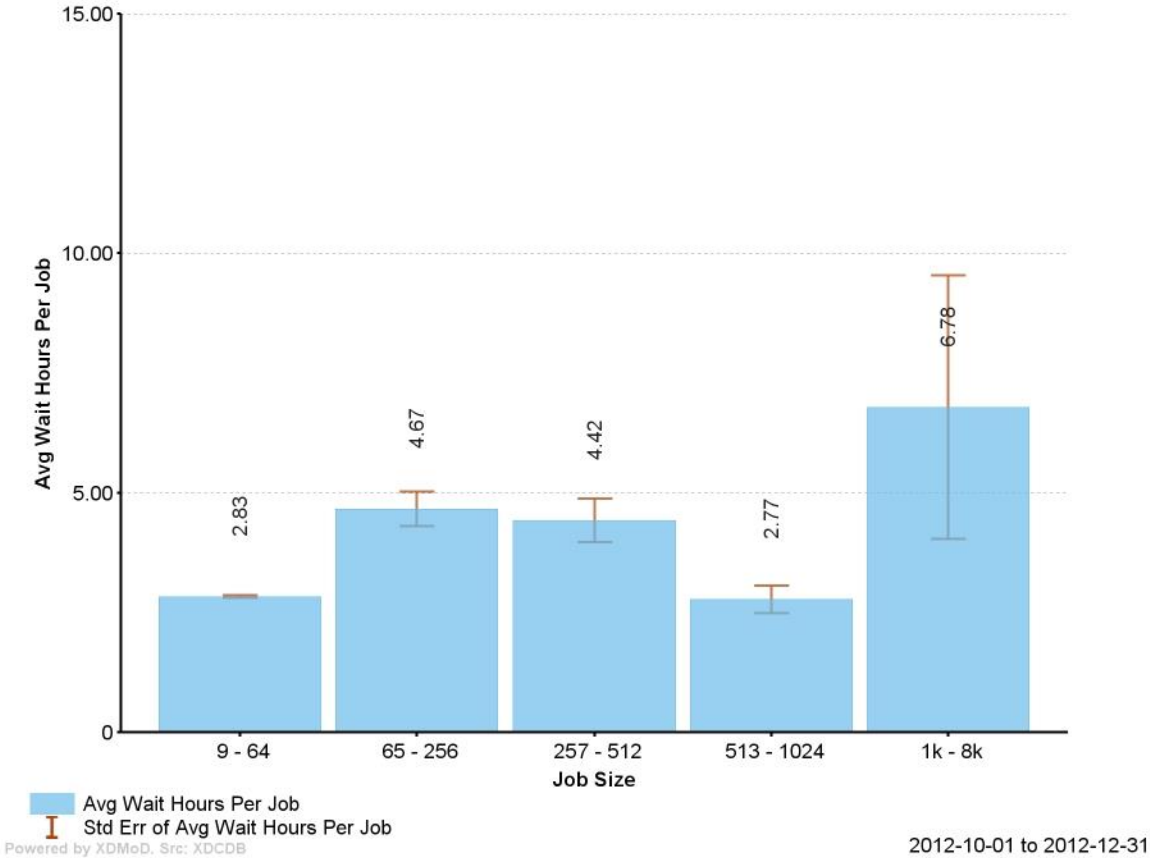
2012-10-01 to 2012-12-31



Avg Wait Hours Per Job by Job Size

Resource = SDSC-GORDON

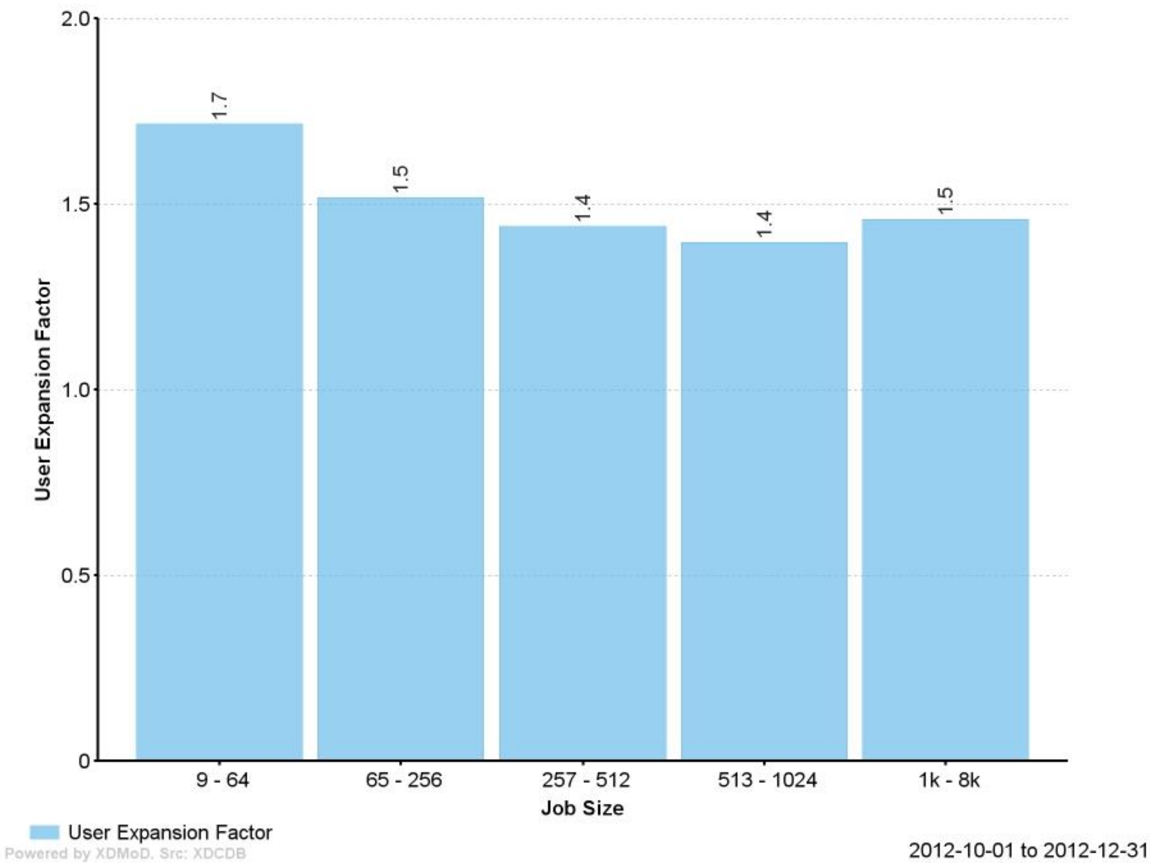
2012-10-01 to 2012-12-31



User Expansion Factor by Job Size

Resource = SDSC-GORDON

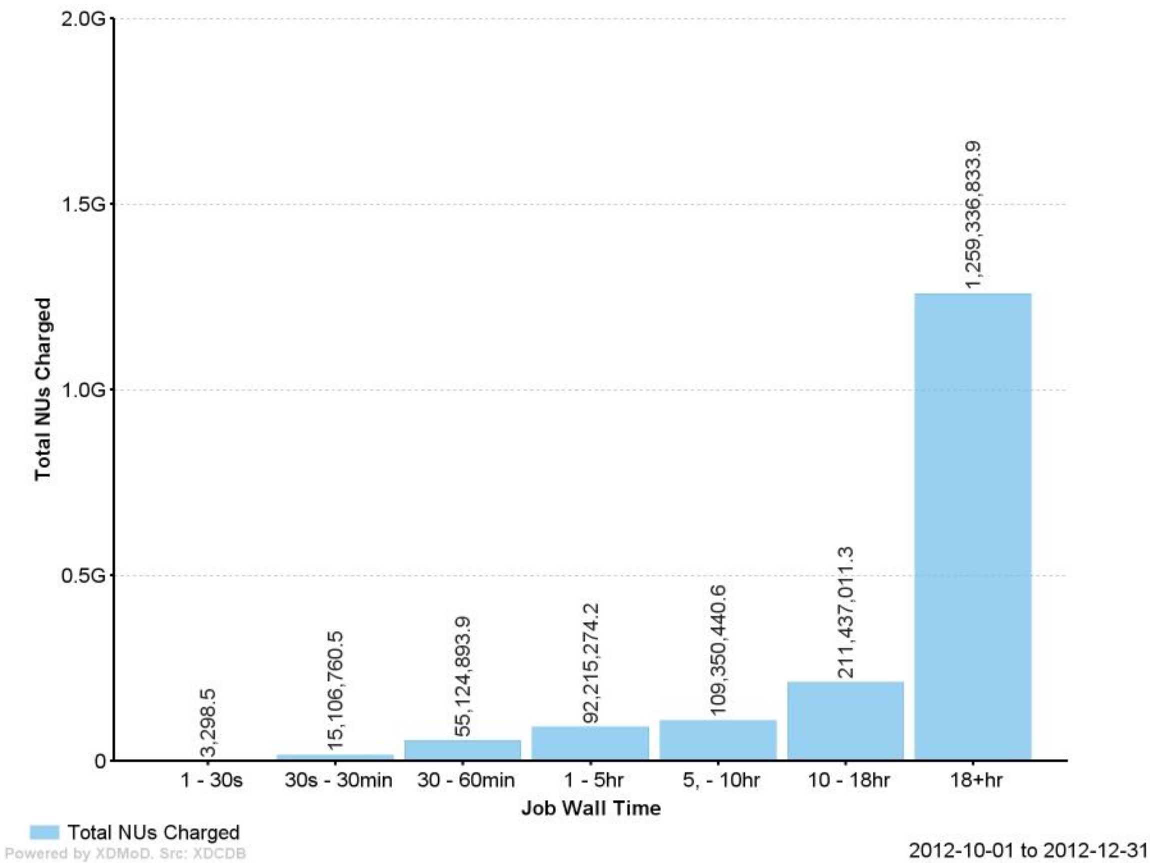
2012-10-01 to 2012-12-31



Total NUs Charged by Job Wall Time

Resource = SDSC-GORDON

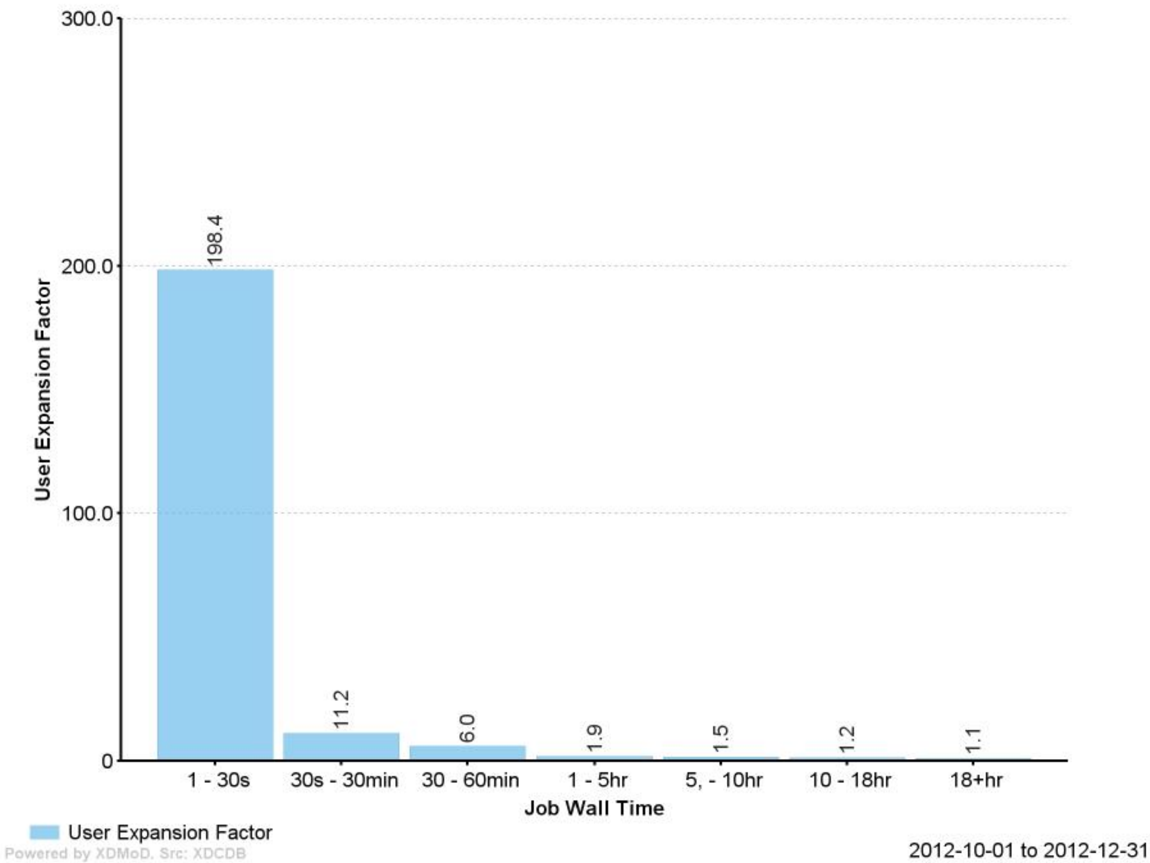
2012-10-01 to 2012-12-31



User Expansion Factor by Job Wall Time

Resource = SDSC-GORDON -- Service Provider = SDSC

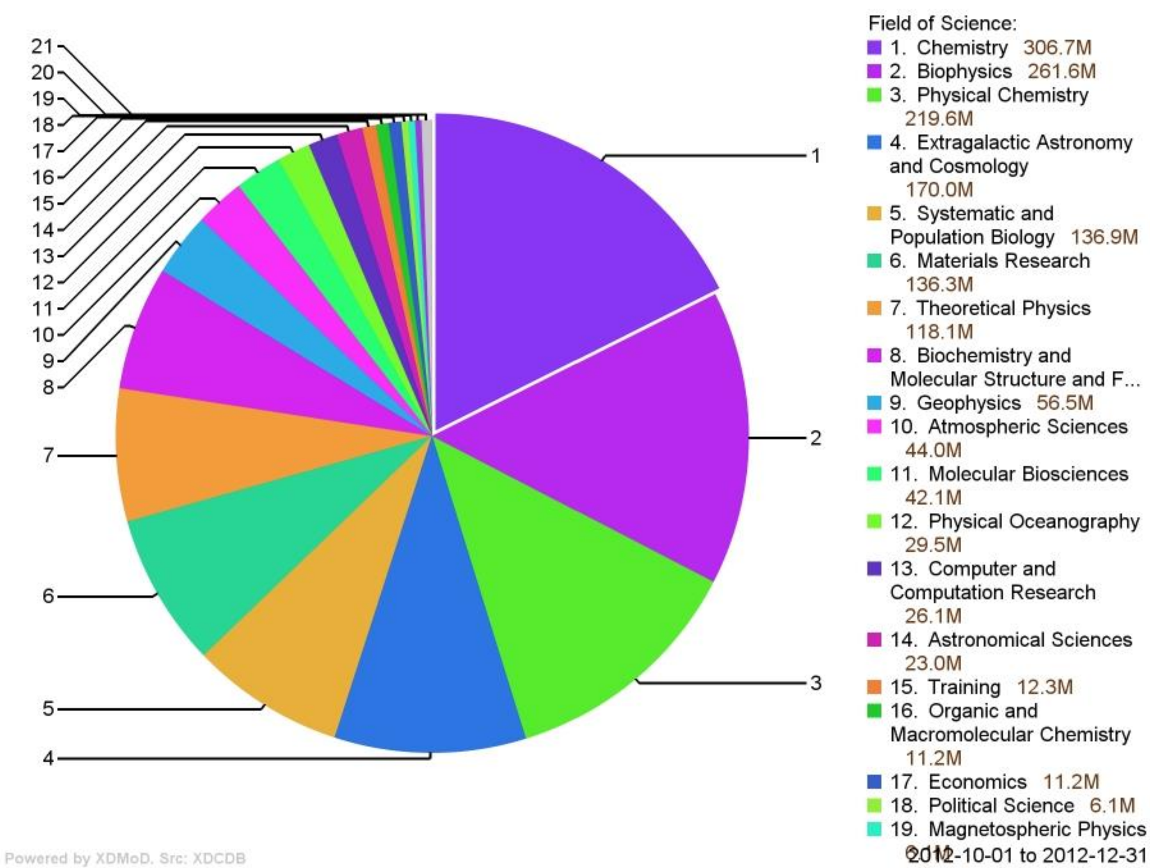
2012-10-01 to 2012-12-31



Total NUs Charged by Field of Science

Resource = SDSC-GORDON

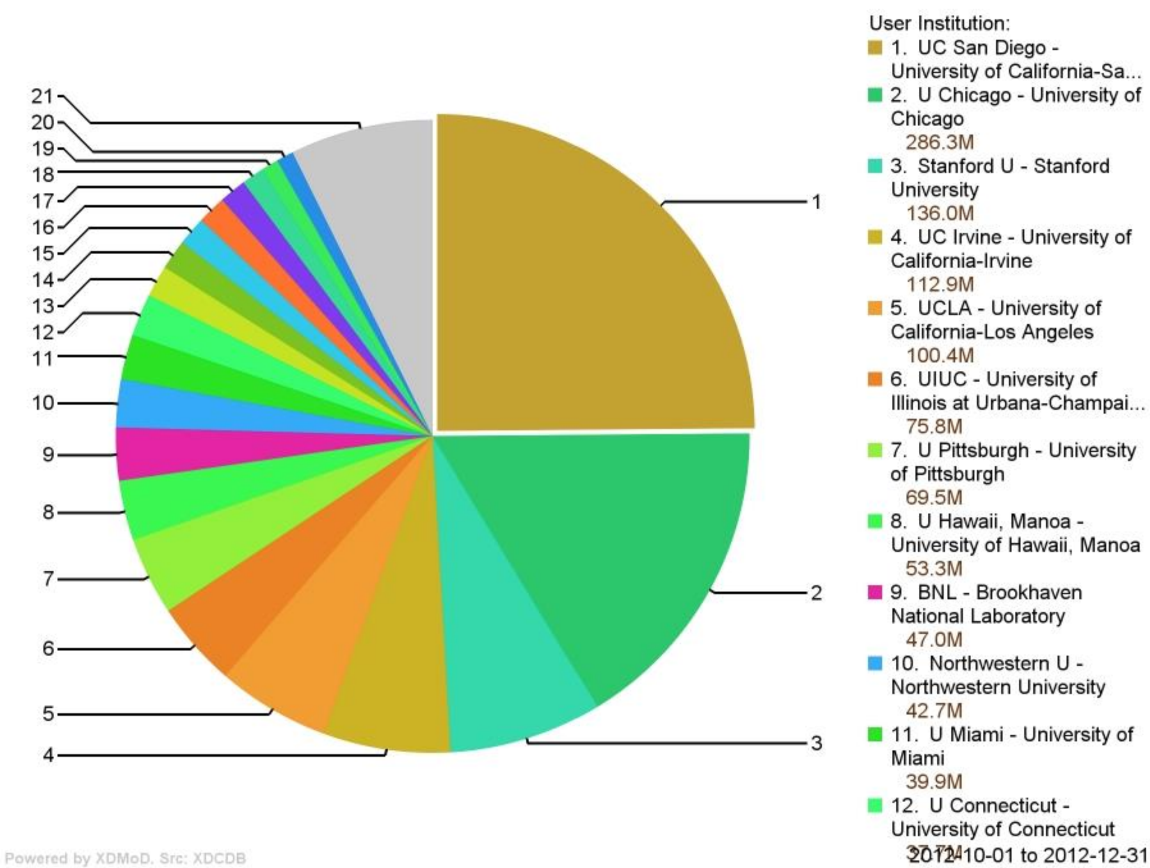
2012-10-01 to 2012-12-31



Total NUs Charged by User Institution

Resource = SDSC-GORDON

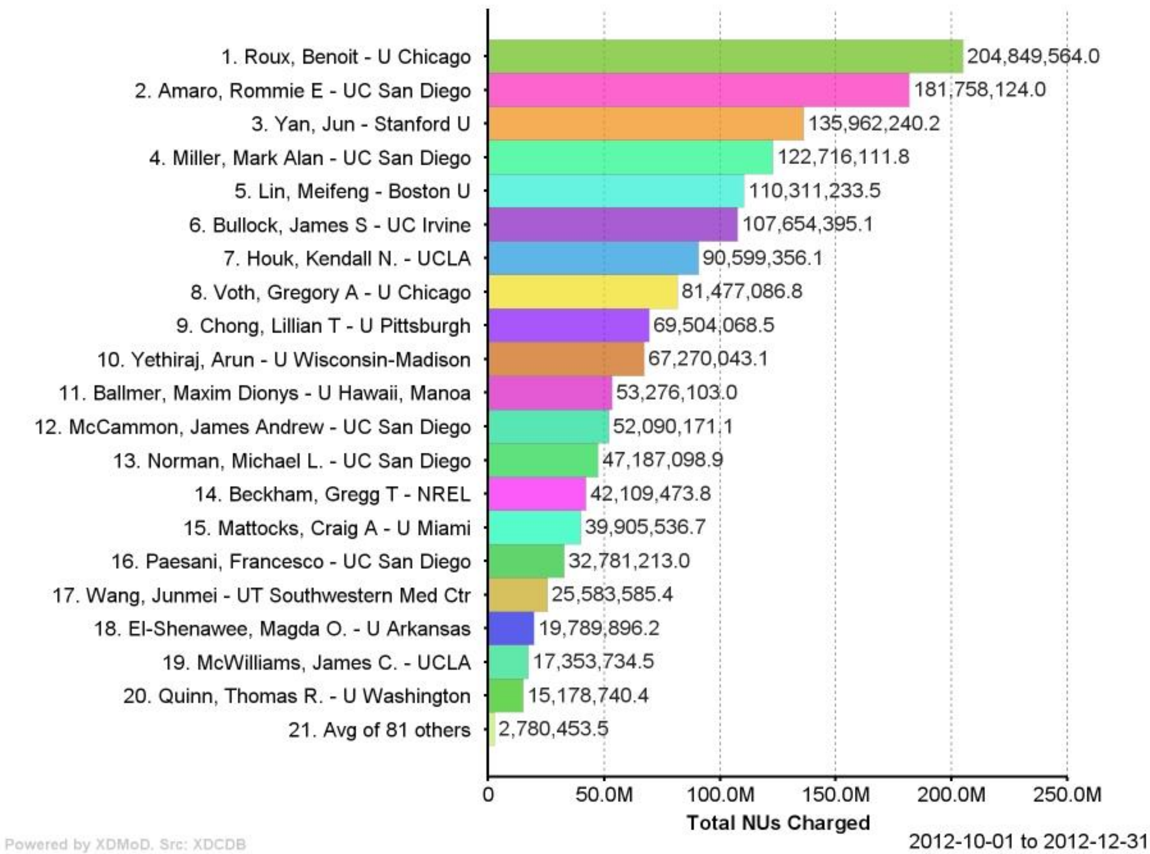
2012-10-01 to 2012-12-31



Total NUs Charged by PI

Resource = SDSC-GORDON

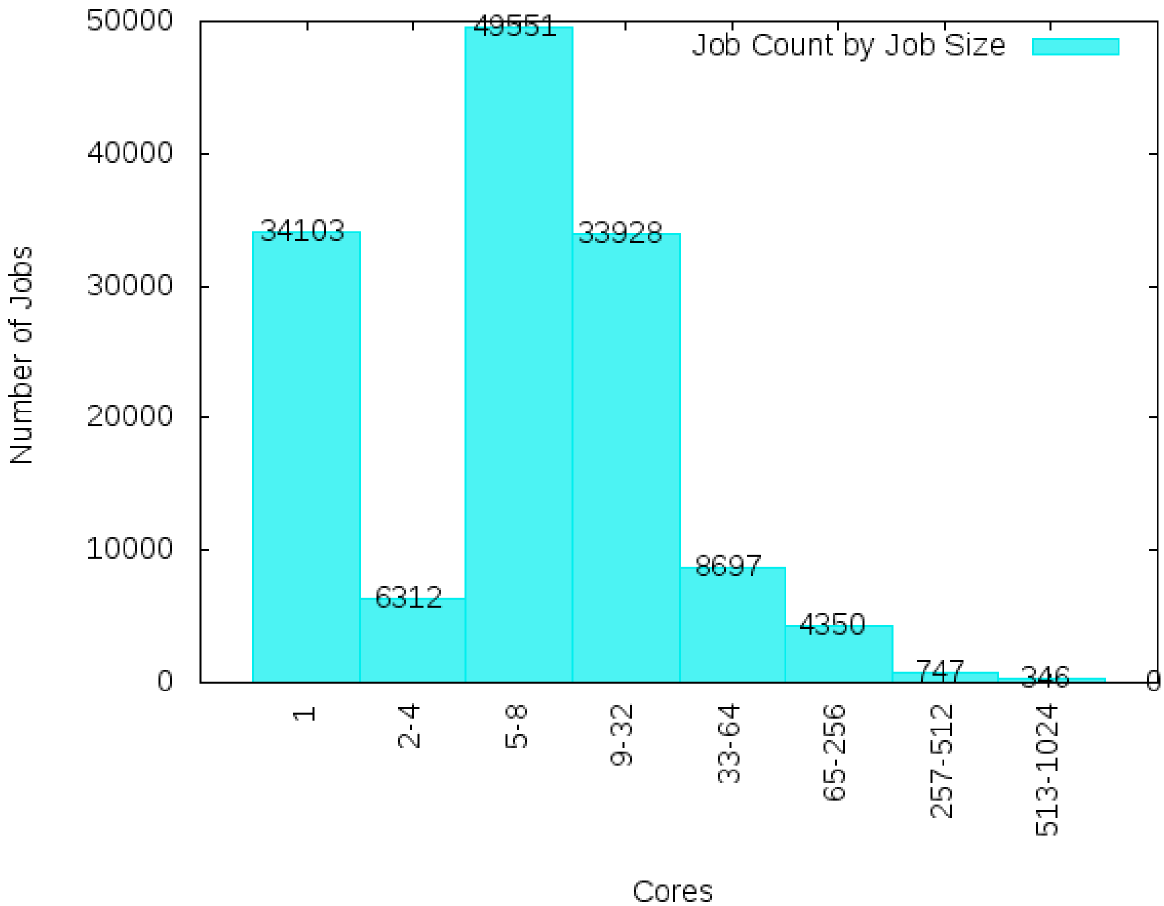
2012-10-01 to 2012-12-31



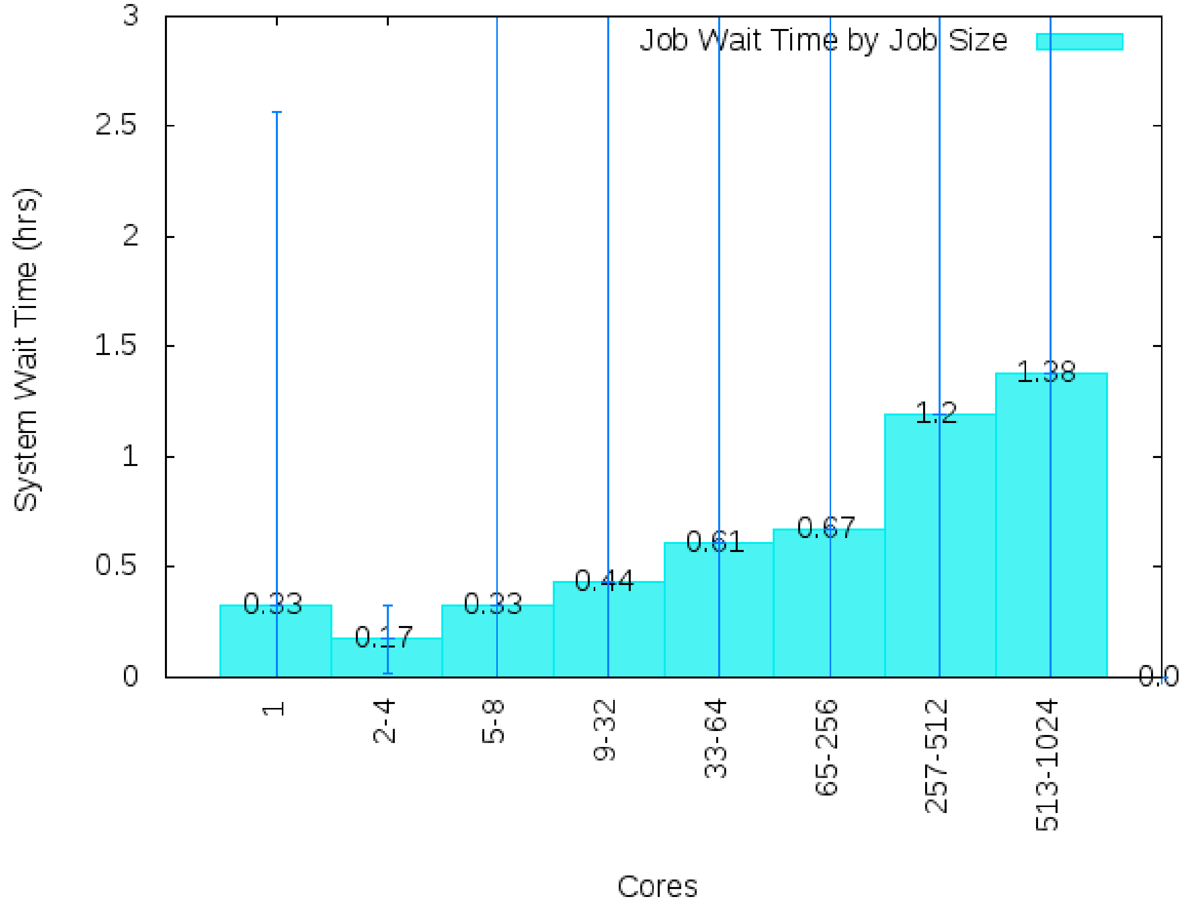
Appendix 1.9C Trestles SP-specific Metrics

2012-07-01 to 2012-09-30

Number of Jobs run by Job Size (Cores)

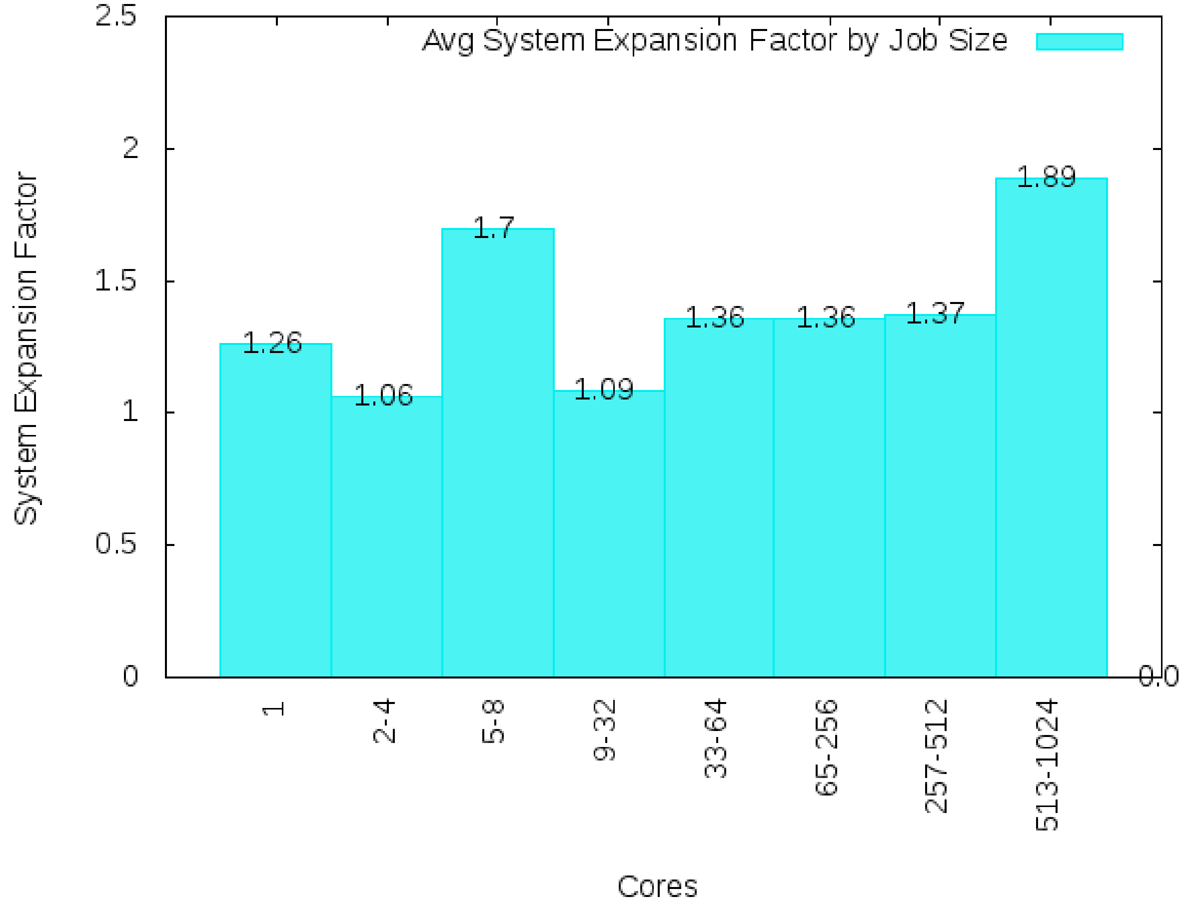


Average System Wait Time (Hours) by Job Size (Cores)

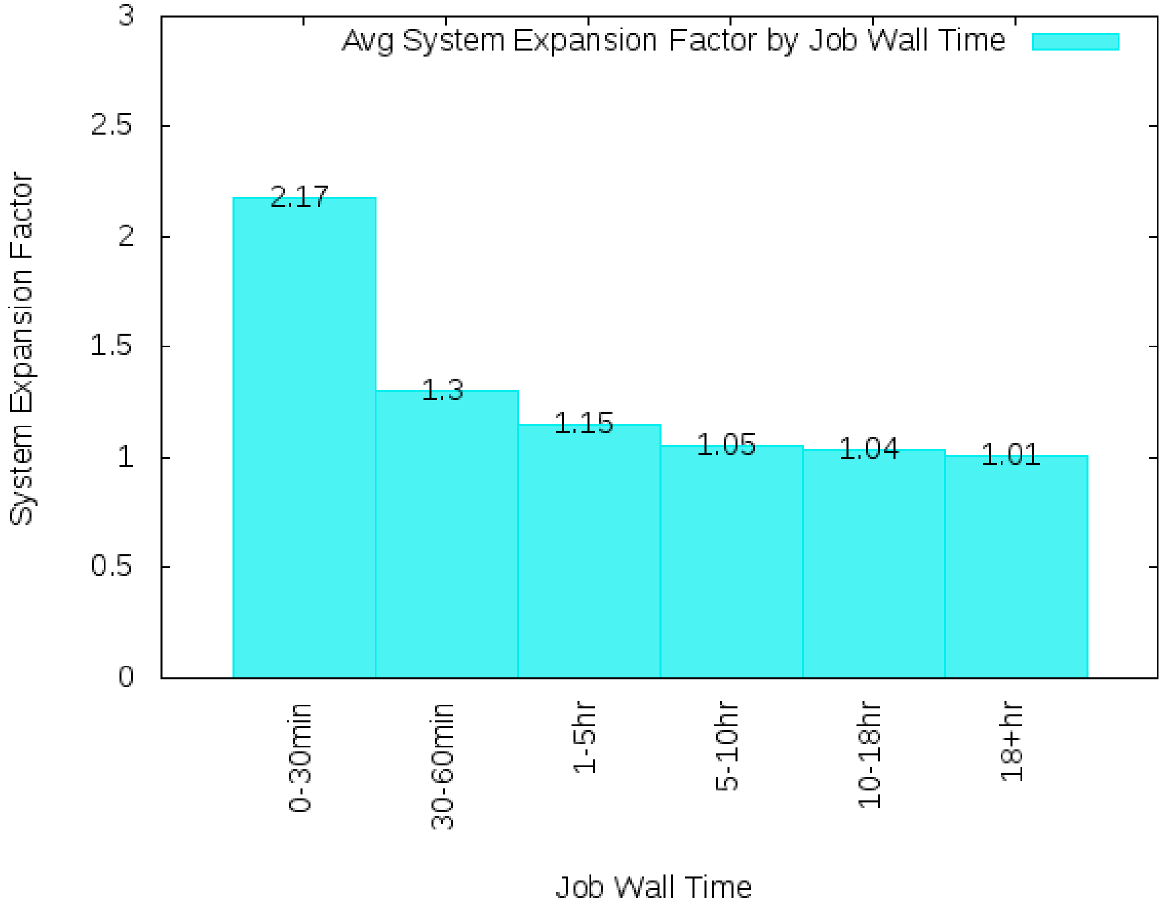


Average Requested Wall Time (Hours) by Job Size (Cores)

Average "Scheduler" Expansion Factor by Job Size (Cores)
(Requested Wall Time + System Wait Time)/Requested Wall Time


Avg System Expansion Factor by Job Size
System Expansion Factor
2.5
2
1.5
1
0.5
0
1.26
1.06
1.7
1.09
1.36
1.36
1.37
1.89
0.0
1
2-4
5-8
9-32
33-64
65-256
257-512
513-1024
Cores

Average Scheduler Expansion Factor by Requested Wall Time (Hours)



20 TACC - Service Provider Quarterly Report

20.1 Executive Summary

The Texas Advanced Computing Center (TACC) at The University of Texas at Austin (UT Austin) develops and deploys an integrated infrastructure of advanced computing resources to enhance the research and education activities of the faculty, staff, and students at UT Austin, and in Texas and across the US through its involvement in various state and national programs, including the NSF funded eXtreme Digital Resources for Science and Engineering (XD) project. This infrastructure includes high performance computing (HPC) systems, advanced scientific visualization (SciVis) systems, data servers and storage/archival systems, grid computing servers, IT systems, high-bandwidth networks, and a comprehensive software environment comprising applications, tools, libraries, databases, and grid software. TACC services include technical documentation, consulting, and training in HPC, SciVis, and grid computing.

TACC staff continued to contribute to the success of the XSEDE project to date. Significant effort was expended in the User Services User Engagement, User Interaction & Interfaces, and Training activities, XSEDE web site, and the Extended Collaborative Support Services area.

TACC continues to take a leadership role in XSEDE training efforts by hosting and/or facilitating 9 training workshops attended by 442 students during the reporting period. The Cornell University team continued to add training modules to and improve the Ranger virtual workshop.

Construction of the new Stampede cluster continued throughout the reporting period. An early user period began in December with 17 major principal investigators and approximately 100 users gaining access to Stampede. Researchers participating in the early user period included 9 XSEDE research groups and approximately 60 XSEDE users. By the end of the reporting period all Sandy Bridge nodes were installed and operational, over 4000 Intel MICs installed, and the entire InfiniBand fabric in place. The system is on schedule for deployment on January 7, 2013.

The Ranger compute cluster, after 5 years as one of the most requested XSEDE resources, is scheduled for decommissioning on February 4, 2013.

20.1.1 Resource Description

Ranger

The TACC Sun Constellation Cluster contains 62,976 cores (2.3 GHz) within 3,936 Sun Constellation blades (nodes), an X4600 Rocks master node, 4 X4600 user login nodes, 4 X4600 user gridftp nodes, 4 X4600 data movers, 2 X4600 nodes dedicated to supporting the SGE batch system, 2 X4600 external management service nodes, 2 X4600 InfiniBand subnet management nodes, an X4100 software build node, and 6 X4600 metadata server nodes to support the Lustre parallel file systems. Multiple work and home file systems are configured from 1.7 PB of storage managed by the Lustre parallel file system management software. Two Sun Data Center 3456 switches are the core of an InfiniBand fabric through which all components are connected. The basic configuration is as follows:

- 3936 Sun Constellation Blade Servers, each with
    - four quad-core 2.0 GHz processors
    - 32 GB of Memory
    - 8 GB flash drive
- 1.7 PB of storage managed by the Lustre Parallel File System software
- InfiniBand Interconnect

Lonestar

The TACC Dell Westmere Cluster contains 22,656 compute cores (3.33 GHz) within 1,888 Dell PowerEdge M610 compute blades (nodes), 15 PowerEdge R610 compute-I/O server-nodes, and 2 PowerEdge M160 login/management nodes. Each compute node has 24 GB of memory, and the login/development nodes each have 24 GB. 14 large memory (1TB) nodes are available for high-throughput computing and applications that require access to a shared-memory architecture and 8 GPU nodes are configured for visualization and applications that can take advantage of the computational speed of the GPUs. The system storage includes a 421 TB parallel WORK Lustre file system, a 841 TB parallel SCRATCH Lustre file system, and 275 TB of local compute-node disk space (146GB/node). A QDR InfiniBand switch fabric interconnects the nodes (I/O and compute) via a fat-tree topology, with a point-to-point bandwidth of 40Gb/sec. The basic configuration is as follows.

- 1888 Dell PowerEdge M610 Blade Servers, each with
  - Dual Intel Westmere 6-core, 3.33 GHz processors
  - 24 GB of Memory
  - 146 GB of Local Disk
- 14 Dell PowerEdge R910 servers, each with
  - Four 6-core, 2.0 GHz Intel Xeon processors
  - 1 TB of Memory
  - 292 GB of Local Disk
- 8 Dell PowerEdge C6100 servers, each with
  - Two NVIDIA M2070 GPUs
  - Two 6-core, Intel Xeon X5670 2.93 GHz processors
  - 24 GB of Memory
  - 146 GB of Local Disk
  - 16-lane PCI Express to Dell C410x PCI expansion box housing the NVIDIA GPUs
- 421 TB Lustre Parallel File System (WORK)
- 841 TB Lustre Parallel File System (SCRATCH)
- QDR InfiniBand Interconnect

Longhorn

The TACC DELL/NVIDIA Visualization & Data Analysis Cluster, Longhorn, is a hybrid CPU/GPU system designed for remote, interactive visualization and data analysis. In addition, Longhorn supports production, compute-intensive calculations on both the CPUs and GPUs via off-hour queues. The large, per-node memory is intended to support serial and parallel visualization and analysis applications that take advantage of large memories, multiple computing cores, and multiple graphics processors. Longhorn is an ideal companion resource for working with large data sets created on Ranger, since Longhorn can directly access Ranger's Lustre parallel file system through a 10 GigE network link.

The system consists of 256 dual-socket nodes, each with significant computing and graphics capability. Total system resources include 2048 compute cores (Nehalem quad-core), 512 GPUs (128 NVIDIA Quadro Plex S4s, each containing 4 NVIDIA FX 5800s), 13.5 TB of distributed memory and a 210 TB global file system. Longhorn configuration details can be found below.

128 NVIDIA Quadro Plex S4s, each with

- 4 NVIDIA FX 5800 GPUs
- 16GB Graphics Memory (4GB per GPU)
- 2 independent graphics busses, one per GPU pair

240 Dell R610 Compute Nodes, each with

- 2 Intel Nehalem quad-core processors (8 cores) @ 2.53 GHz
- 48GB RAM
- 73GB local disk
- connected to 2 dedicated NVIDIA FX 5800 GPUs via Quadro Plex graphics bus

16 Dell R710 Compute Nodes, each with

- 2 Intel Nehalem quad-core processors (8 cores) @ 2.53 GHz
- 144GB RAM
- 73GB local disk
- connected to 2 dedicated NVIDIA FX 5800 GPUs via Quadro Plex graphics bus

Mellanox QDR InfiniBand Interconnect

14 Dell PowerVault MD1000 Direct Attached Storage Arrays (210TB global file system, managed by the Lustre Parallel File System)

Spur

TACC's Terascale Sun Visualization Cluster contains 128 compute cores, 1 TB aggregate memory and 32 GPUs. Spur acts not only as a powerful stand-alone visualization system: it also enables researchers to perform visualization tasks on Ranger-produced data without migrating to another file system and to integrate simulations and rendering tasks on a single network fabric. The cluster consists of the following hardware:

- 1 Sun Fire X4600 server with 2 NVIDIA Quadro Plex model 4. The X4600 contains 8 dual-core CPUs (16 cores total) and 256GB of RAM. Each Quadro Plex model 4 contains 2 NVIDIA Quadro FX5600 GPUs;
- 1 Sun X4400 servers, with 4 quad-core CPUs (16 cores total) and 128GB of RAM, connected to 2 NVIDIA Quadro Plex model 4. Each Quadro Plex model 4 contains 2 NVIDIA Quadro FX 5600 GPUs;
- 6 Sun X4400 servers, each with 4 quad-core CPUs (16 cores total) and 128GB of RAM, and each connected to an NVIDIA Quadro Plex S4. Each Quadro Plex S4 contains 4 NVIDIA Quadro FX 5600 GPUs; and
- Total system capability: 128 cores, 1TB aggregate memory, 32 GPUs.

Because Spur shares Ranger's interconnect fabric and file systems, researchers will be able to easily transition between HPC runs to generate and visualize data. Furthermore, visualization software is able to harness both the rendering power of the graphics hardware and the compute power of Ranger to enable the analysis of terascale and larger data sets.

20.2 Science Highlights

Chemistry: Investigation of the Origin of Catalytic Activity in Oxide-Supported Nanoparticle Gold (PIs: Wenjie Tang, University of Virginia)

Aaron Dubrow (aarondubrow@tacc.utexas.edu)

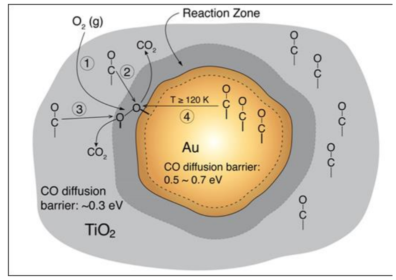


Figure n. Schematic of the mechanism of low temperature CO oxidation over an Au/TiO2 catalyst at a perimeter zone of reactivity. CO molecules on the TiO2 can be oxidized at the perimeter site at a temperature as low as 120 K, as shown in the processes 2 and 3. (*Science*, vol. 333 no. 6043 pp. 736-739. DOI: 10.1126/science.1207272)

Because of its ability to split strongly bonded molecules, gold titanium-oxide nanocatalysts are a leading candidate for industrial applications that use biomass or fuel cells to create clean energy. In these nanocatalysts, minute particles of gold dot the surface of titanium-oxide. The forces that emerge from the combination of these two materials are strong enough to break the O-O bond of oxygen molecules and the C-O bond of acetic acid, a byproduct of biomass conversion that, when combined with hydrogen, forms ethanol, an important precursor for fuel. Researchers knew that metal nanoparticles supported on an oxide surface have high catalytic activity for a variety of reactions, but how this process worked, and the locations of its active sites, was not well understood. Combining laboratory experiments and computer simulations on the Ranger supercomputer, an XSEDE-allocated resource, Wenjie Tang, a research associate in the department of chemical engineering at the University of Virginia, discovered a reaction site on the perimeter of the gold-titanium complex where much of the catalytic activity occurs. Her initial findings were reported in the August 2011 edition of *Science* and further results of the study were published in the June 2012 edition of *the Journal of the American Chemical Society (JACS)*. In the August 2012 edition of *JACS*, Tang and her teammates reported the first catalytic oxidation of acetic acid to ketenylidene (CCO) over a gold titanium-oxide catalyst. (Oxidation is the loss of electrons by a molecule — an important process for catalysis.) The researchers believe the discovery of this intermediate product, ketenylidene, will lead to the creation of valuable hydrocarbon fuels via reactions such as Fischer-Tropsch process. Catalytic reactions happen fast and the intermediate structures that form are not always apparent in the experimental process. Computer simulations allow scientists to slow down the reactions in order to uncover and visualize the forces acting on molecules at the atomic level. The researchers used the Ranger supercomputer to explore aspects of the material reaction at the nanoscale that could not be investigated in the laboratory. Using density functional theory, the researchers calculated the quantum mechanical interactions of more than 200 atoms. The simulations helped the group identify the presence of an intermediate chemical in the reaction and determined that it was in fact ketenylidene. The acetic acid-to-ketenylidene path is "a crucial step for biomass conversion into more valuable industrial chemicals," the authors wrote.

Molecular and Cellular Biosciences: Simulations of DNA damage and repair processes (PI: Suse Broyde, New York University)

Aaron Dubrow (aarondubrow@tacc.utexas.edu)

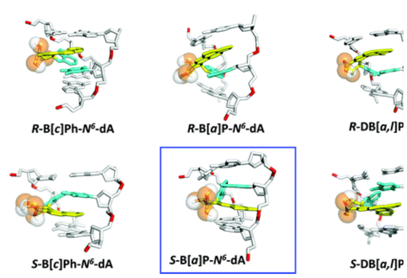


Figure n. Models showing the steric hinderance between different lesions (colored yellow and turquoise)and DNA. Steric hinderance causes double helix destabilization and refers to the degree of crowding between different atoms.

A person doesn't have to go far to find a polycyclic aromatic hydrocarbon (PAH). These carcinogen precursors are inhaled through automobile exhaust during the morning commute, are present in cigarette smoke, and are part of any barbequed meal. Once ingested or inhaled, the multi-ringed molecules are converted into reactive carcinogenic compounds that can bind to DNA, sometimes literally bending the double helix out of its normal shape, to form areas of damage called lesions. The damaged DNA can create errors in the genetic code during replication, which may cause cancer-initiating mutations. It is the job of the nuclear excision repair (NER) system to repair damage caused by PAH lesions by removing the segment of DNA where the lesion is bound and patching up the resulting gap. But some lesions are especially resistant to this repair machinery, making them more likely to cause mutations. A research team at New York University (NYU) has gained new insights into the ability of certain PAH-derived lesions to evade the DNA repair machinery. Through simulations and visualizations on XSEDE-allocated resources, they found that some lesions stabilize the DNA they damage, making it difficult for a certain repair protein to mark the lesion for repair. Their research was published earlier this year in the February 2012 issue of *Biochemistry* and further articles about NER and DNA lesions appeared in *Nucleic Acids Research* in July and August. The stability of the DNA double helix is a key feature that determines whether DNA is flagged for repair in the first place by a protein called XPC. The protein patrols the genome looking for weakened areas. When it finds weak spot, it slips a structure called a beta-hairpin between the strands, marking the DNA for NER. But if a lesion makes DNA more stable, the strands become more difficult to separate and the beta hairpin can't signal for repair. Broyde and her team examined six different lesions types (caused by three chemicals with two different geometric configurations each). The simulations revealed that those caused by dibenzo[a,l]pyrene, the most tumorigenic PAH investigated, were the most resistant to repair. The five-ringed structure of the carcinogen provided ample stacking opportunities, which stabilized the DNA much better than the four and three-ringed structures of the other PAHs that were examined. Knowing which lesions are the most repair-resistant could play an important role in preventative medicine, said Broyde, as individuals harboring them could be counseled to avoid further exposure, particularly in the case of smokers.

Longhorn/Spur

The top five users on Longhorn and Spur this past quarter were:

1. Michael Hagan, Brandeis University, computing simulations of viral capsid assembly at multiple resolutions
2. Dmitry Matyushov, Arizona State University, computing the energetics of natural photosynthesis
3. Chuan Xiao, University of Texas at El Paso, computing cryo-EM reconstruction of the giant marine virus CroV
4. Robert Sugar, University of California, Santa Barbara, computing lattice gauge theory on MIMD parallel computers
5. Dean Corbae, University of Texas at Austin, Department of Economics, computing mortgage innovation and the foreclosure boom

The work conducted by Dr. Corbae’s group proves particularly interesting and presents a model where heterogeneous households select from a set of possible mortgage contracts and choose whether to default on their payments given realizations of income and housing price shocks. The mortgage menu consists of fixed rate mortgages (FRM) which require a 20% downpayment as well as mortgages with low downpayment and non-traditional amortization schedules which became popular after 2004. The mortgage market is competitive and each contract, contingent on household earnings and assets at origination as well as loan size, must earn zero expected profits. Simulations calibrated to pre-2004 US data identify important selection effects associated with the introduction of non-traditional mortgages which enable households with low income and assets to become homeowners. At the same time, average default rates rise precisely because households with characteristics which make them more likely to default enter the mortgage market and because households accumulate equity earlier when they hold FRMs than when they hold mortgages with low initial payments. Dr. Corbae and his group compute the model to quantify the role of mortgage innovation in the recent rise in foreclosure rates by shocking the economy with an unanticipated aggregate decline in houses prices after briefly introducing a non-standard mortgage option.

Ranger and Lonestar

Plants grow with their leaves toward the sun and their roots toward the ground. It has long been thought this was due to sunlight, but it even happens inside a dark box. Patrick Mason at the University of Wisconsin-Madison, a user in the iPlant project, is using Ranger to determine how plants respond to gravity (“gravitropism”). A big data problem, this investigation begins with 1.8 billion RNA sequence reads, which are then analyzed to determine which gene networks are active as plant growth changes direction in response to gravity. The team worked with TACC and iPlant staff to adapt their pipelines to Ranger.

Different species of Buffalo are critical sources for milk and food in much of the world. Genotyping Buffalo has been challenging, however, since these animals are primarily important in developing countries, and as such, a major investment in a reference genome has never been made. In conjunction with the iPlant project and TACC, Jim Reecy’s team at Iowa State University has used Lonestar and the iPlant Discovery Environment to design an assay using the reference genome for cattle that will allow cheap and easy measurement of diversity for Buffalo. Enabling an affordable assay will allow breeders to apply many of the techniques used to improve cattle to be used with Buffalo around the world.

At UC-Davis, researcher’s in Neelimha Sinha’s lab used the iPlant Discovery Environment and the Ranger system to BLAST and annotate 400,000 transcripts against the NCBI NR (non-redundant) database in just 24 hours. Using up to 2,048 cores of Ranger, this workflow formally took this lab two months on local cluster resources (and the assistance of trained bioinformatics staff to build the command lines). The resulting data, from species such as ferns, cycads, and other angiosperms is being used to understand how leaves evolved.

20.3 User-facing Activities

20.3.1 System Activities

20.3.2 Services Activities

20.4 Security

There have been no changes in TACC security procedures or security incidents/responses within the reporting period.

20.5 Education, Outreach, and Training Activities

TACC Outreach Activities

XSEDE Education and Outreach activity in Q4CY2012 continued with participation in bi-weekly Outreach reporting and planning conference calls, Underrepresented Outreach reporting and planning conference calls on alternate bi-weeks, and monthly TEOS all calls.

Planning continued with Linda Akli from SURA and Pat Teller from UTEP to present the first XSEDE Regional Workshop west of the Mississippi. February 19 and 20, 2013 were decided on to coincide with the inauguration of UTEP’s expanded computing for academic research initiative. Planning for 50 plus participants was started with pre-surveys of interest indicating up to 90 participants showing interest in a scientific computation workshop. Registration for the conference opened in December.

Outreach to cohort groups continued with TACC’s External Relations team developing the first domain specific XSEDE information sheet for use at a targeted event. The information sheet was developed by TACC’s science writer, Aaron Dubrow, and web-administrator, Hedda Prochaska and focused on the chemistry domain. The information sheet about XSEDE resources supporting computational chemistry was used by SURA at the National Organization for the Professional Development of Black Chemist and Chemical Engineers (NOBCChe) annual conference in Washington, D.C. September 25-28.

Outreach also continued with TACC representing XSEDE at the 19th Annual Institute on Teaching and Mentoring, October 25-28 in Tampa, Florida. The invitation-only conference was attended by over 900 graduate students, post-docs, and faculty, with the majority of students coming from Minority-Serving Institutions. Conference participants were all affiliated with diversity initiatives, including the NSF Alliance for Graduate Education and the Professoriate, NIH Bridges to the Doctorate, Federation of American Societies for Experimental Biology, Gates Millennium Scholars, Ronald E. McNair Postbaccalaureate Achievement Program, New England Region Scholars, Alfred B. Sloan Foundation Minority Ph.D. Program and the Southern Regional Education Board Doctoral Scholars Program. More than 100 contacts were made and several opportunities were identified for offering XSEDE training. Based on participant feedback at the conference, the Institute has already invited XSEDE to attend in 2013.

The original invitation resulted from participation in another XSEDE outreach initiative in Q2CY2012, the NSF Joint Administrative Meeting. Follow ups continued in Q4CY2012 with contacts from the highly productive assortment of networking activities at the National Science Foundation Joint Administrative Meeting in Q2CY2012 in Washington, D.C. for Principal Investigators in the EHR Directorate.

The Campus Champion discussion with Austin Community College (ACC), a two-year college in Austin, Texas was jumpstarted in Q4CY2012 with the visit of a task force from ACC visiting TACC's visualization lab in an effort to identify opportunities for collaboration between TACC and ACC's Student Success Initiative. The visit was coordinated by TACC's Community Engagement Coordinator and was lead by the Assistant Vice President for Student Initiatives at ACC accompanied by the Dean for Computing Studies and Learning Technologies, the Chair of Computer Studies, and other STEM faculty.

The Austin Forum on Science, Technology & Society

In the reporting period, TACC hosted a total of 3 monthly Austin Forum events with invited speakers from areas of interest focusing on science and technology. The goal of The Austin Forum on Science, Technology & Society is to engage and educate the local community about the numerous ways in which science and technology enhance the quality of their everyday lives, as well as the health, prosperity and security of the nation. One hour is devoted to a presentation and Q&A discussion between the speaker and guests. Ample time for networking is offered, both preceding and following the speaker presentation. The speaker series has become increasingly popular in the community, attracting a total of 575 people this quarter. This quarter, the speaker series included Dr. Doris Taylor, a world-renowned American scientist known for her achievements in research and decellurization, as well as Dr. John (Jay) Boisseau, Director of TACC.

TACC Facility Tours and Presentations

From K-12 and higher education groups, and special populations including senior citizens, TACC conducted facility tours and outreach presentations impacting 632 people in Q4CY2012, over half who were under-represented and participants of the Pre-College Academic Readiness Program (PCARP), led by the UT Division of Diversity and Community Engagement. PCARP participants attend Title 1 (underperforming schools) throughout the state of Texas. An overview of XSEDE and TACC were given at each event.

Type	Title	Location	Date(s)	Number of Participants	Number of Under-represent ed people
The Austin	*"More Than You*	AT&T	10/2/12	265	Not

Forum on Science, Technology and Society	*Think You Know: Analyzing the Data That's Around Us"* w/John B. Gordon	Conference Center			tracked.
Vislab Tour	**UT ECE and CS Undergrad students: Paul**	Vislab	10/2/12	20	Not tracked.
Vislab Tour	**UTeach PBI course-undergraduate and graduate students**	Vislab	10/4/12	8	5
Vislab Tour	**Bastrop ISD: Cedar Creek & Bastrop HS (seniors)**	Vislab	10/5/12	30	15
Vislab Tour	**PCARP-**high school students Lanier-Austin & Travis High Schools	Vislab	10/11/12	160	160
Machine Room Tour	**VIP Tour: Dell**/Potosino de Investigacion Cientifica y Tecnologia	Vislab	10/18/12	5	5
Vislab Tour	**UT ECE FIG: Bits and Bytes, freshmen**	PRC	10/23/12	25	Not tracked.
Vislab Tour	**UT ECE FIG: Bits and Bytes, freshmen**	AT&T Conference Center	10/24/12	25	Not tracked.
Vislab Tour	**UT ECE FIG, freshmen**	Vislab	10/24/12	26	Not tracked.
Vislab Tour	**UT Learning Technologies-freshmen**	Vislab	10/25/12	20	Not tracked.
Vislab Tour	**UTeach PBI students and high school students**	PRC	10/27/12	40	Not tracked.
Vislab Tour	**UT ECE FIG, freshmen**	PRC	10/29/12	30	Not tracked.
Vislab Tour	**PCARP Chem Bridge- UT Outreach Houston/Dallas high school**	Sun City	10/30/12	88	88

	students				
Machine Room Tour	The Institute of Classical Archaeology	PRC	10/31/12	7	4
Vislab Tour	**VIP: Cockrell**	PRC	11/1/12	3	1
Machine Room Tour	**VIP: Dell Enterprise Group**	AT&T Conference Center	11/6/12	8	0
Vislab Tour	**UT ME FIG, freshmen**	PRC	11/7/12	32	32
The Austin Forum on Science, Technology and Society	***"Solutions for Heart Disease: The Science of the Future Today"* *w*/Doris Taylor**	AT&T Conference Center	11/8/12	178	Not tracked.
Machine Room Tour	**Danish Defense**	Vislab	11/8/12	8	2
Vislab Tour	**UT EE FIG, freshmen**	Vislab	11/8/12	21	Not tracked.
Vislab Tour	**VIP: MCCombs School Advisory Council (spouses)**	PRC	11/9/12	30	30
Vislab Tour	**UT FIG Newton, freshmen**	PRC	11/14/12	17	Not tracked.
Vislab Tour	**VIP: Dell University of Chile**	Sun City	11/21/12	7	7
Vislab Tour	**Leander Middle School**	PRC	11/21/12	4	2
Vislab Tour	**VIP: ACC**	PRC	11/27/12	6	3
Vislab Tour	**UT SURGe**	AT&T Conference Center	11/29/12	4	2
Machine Room Tour	**Dell Product Engineers**	PRC	11/30/12	8	0
The Austin Forum on Science, Technology and Society	"Enabling Discoveries w/Digital Data, Supercomputing and Vis" w/Jay Boisseau, Patti Hurn, Matt Vaughn, and Jim Bankson	AT&T Conference Center	12/4/12	132	Not tracked.

TACC Education and Training Activities

Scientific Computing Curriculum and Courses

Several of TACC's Fall 2012 courses were waitlisted as classes continue to grow and students in the academic courses continued expressing interest in additional training courses offered at TACC. Fall enrollment scientific computing course totals were 27 graduate students and 49 undergraduates. Courses being taught by TACC staff include: Introduction to Scientific Programming (9 graduate students and 20 undergraduates), Scientific and Technical Computing (12 graduates and 16 undergraduates), and Visualization and Data Analysis (6 graduate students and 13 undergraduates). Students in the introduction to Scientific Programming and Scientific and Technical Computing classes were assigned accounts on *Ranger*. Students in the Visualization and Data Analysis class were assigned accounts on *Longhorn*.

The courses are offered in the Flawn Academic Center in a customized classroom housing both lecture space and a computer instruction laboratory. The classroom customization was made possible through a partnership with Chevron to increase instruction in scientific computing.

The partnership with the UT Austin Division of Statistics and Scientific Computation (DSSC) continued with DSSC being the home of the Scientific Computation courses. DSSC offers an Undergraduate Certificate and a Graduate Portfolio Program in Scientific Computation, both commonly being referenced as the certificate program. TACC meet with the certificate program's faculty advisory council to provide input on what should count for credit for scientific computation, as increased student interest in the certificate across disciplines is requiring greater clarification as to what courses encompass a scientific computation preparation. Four of the scientific computing classes taught by TACC fulfill requirements for the certificate and portfolio. The advisory group recognized the appropriateness of the TACC taught intro classes to scientific computation and recommended that they become the required courses for computing, versus the current menu of computation based classes offered across disciplines. Documentation of students completing the certificate program appears on their transcript as a notation. As of Q4, 11 students have completed the program since its inception. For Q4CY2012, 50 students are enrolled in the program. Enrollment in the certificate program includes 48% from the College of Natural Science (which is home to mathematics, statistics, and computer science), 28% from the Cockrell School of Engineering, 16% from the College of Liberal Arts, and 8% from the McCombs School of Business. DSSC's scientific computing course descriptions are online at:

http://www.tacc.utexas.edu/education/academic-courses

Longhorn PI, Kelly Gaither, has developed a short course that will be piloted in May at the Summer Statistics Institute at The University of Texas at Austin. Additionally, PI Gaither gave the keynote at the High Performance Graphics conference on Longhorn and future large-scale visualization platforms.

Training

TACC staff conducted and/or facilitated 9 training workshops/tutorials with the reporting period. A total of 442 attended these training events either in person or via webcast. Most workshops were recorded and a link to the recording provided to attendees for later viewing or to pass on to colleagues. The following table lists the date, title, location and attendance for each event.

Type	Title	Location	Date(s)	Hours	Number of Participants	Number of Under-represented people	Method
Wkshp	Computational Biology	UT Austin	10/8/12	5	40	16	S
Tutorial	HPC Python Tutorial	TACC	10/15/12	7	151	13	S

Wkshp	Intro to Parallel Computing on Lonestar	TACC	10/22-23/12	16	34	7	S
Wkshp	Using Corral for Research Data Management	TACC	10/25/12	3	40	9	S
Wkshp	XSEDE New User Training	TACC	10/26/12	1.5	57	9	**S**
Wkshp	Ranger to Stampede Transition	Cornell	11/6/12	16	19	2	S
Tutorial	Stampede Tutorial	SC12	11/12/12		21	3	S
Wkshp	Ranger to Stampede Transition	Cornell	12/11/12	16	28	4	S
Wkshp	Writing a Successful XSEDE Allocation Proposal	PSC – facilitated by TACC	12/12/12	1	52	12	S

The Virtual Workshop provides users access to twenty-seven training modules with new modules under development and existing modules being reviewed for updates. Users who are logged in to the XSEDE portal can pass-through to the Virtual Workshop, or they can use guest registration.

Available Modules

Programming Languages
An Introduction to Linux
An Introduction to C Programming
An Introduction to Fortran Programming
An Introduction to Python
Python for High Performance
Balancing Scripts and Compiled Code in Scientific Applications
MATLAB Programming

Parallel Computing
Parallel Programming Concepts and High-Performance Computing
Ranger Environment
Message Passing Interface (MPI)
MPI Point-to-Point Communication
MPI Collective Communications
MPI One-Sided Communication
MPI Advanced Topics
Parallel I/O
OpenMP Hybrid Programming with OpenMP and MPI

Code Improvement

Profiling and Debugging
Optimization and Scalability Series Part 1: Planning for Parallel
PerfExpert
Computational Steering
Use Cases

Data Analysis
Large Data Visualization
Paraview
VisIt
Using Databases
MapReduce

Modules Currently under Development
Allocations
Data Transfers
R
Transition to Stampede
MATLAB PCT, MDSC, and MEX
Optimization and Scalability, parts 2 & 3
Advanced Batch
SLURM

Table: Virtual Workshop Usage

	Page Loads	Unique Visitors	First Time Visitors	Returning Visitors
Q1 '11	4,456	920	730	190
Q2 '11	16,281	2,988	2,509	479
July – Sept 2011	9,208	2,905	2,457	448
Oct – Dec 2011	10,068	3,615	3,019	596
Jan – Mar 2012	16,800	5,318	4,249	1069
Apr – Jun 2012	17,875	5,860	4,795	1,065
July – Sept 2012	23,888	5,611	4,442	1,169
Oct – Dec 2012	20,473	7,093	5,649	1,444

Note: the Q2 '11 numbers were a result of high activity after an online news release on the Virtual Workshop was sent out.

20.6 SP Collaborations

Longhorn PI, Kelly Gaither, continutes to collaborate with Purdue University and the RVAC visual analytics center led by Co-PI Ebert. Additionally, collaborations with Co-PIs at The University of Utah and at NCAR. PI has initiated several additional collaborations with institutions in a number of the EPSCoR states, including Hawaii, South Carolina and Utah.

20.7 SP-Specific Activities

20.8 Publications

Harrison C., Navrátil P., Moussalem M., Jiang M., Childs H. "Efficient Dynamic Derived Field Generation on Many-Core Architectures Using Python" *Proceedings of Workshop on Python for High Performance and Scientific Computing (PyHPC) 2012. November 16, 2012*

Navrátil P., Barth W., Childs H. "Virtual Rheoscopic Fluids for Dense Large-Scale Fluid Flow Visualizations" *Proceedings of IEEE Symposium on Large Data Analysis and Visualization (LDAV) 2012. October 14-15, 2012*

Johnson J., Abram G., Westing B., Navratil P., Gaither K. "DisplayCluster: An Interactive Visualization Environment for Tiled Displays" *Proceedings of IEEE Cluster 2012*

Arora R., Bangalore P., Mernik M. "Techniques for Non-invasive Explicit Parallelization" *Journal of Supercomputing, 62/3/1583-1608*

Kuhn V., Craig A., Arora R., Bock D., Cai D., Franklin K., Marini L., Simeone M. "Large Scale Video Analytics: On-demand, Iterative Inquiry for Moving Image Research" *eScience 2012*

Kuhn V., Craig A., Arora R. "Multiple Concurrent Queries on Demand: Large Scale Video Analysis in a Flash Memory Environment as a Case for Humanities Supercomputing" *XSEDE '12 Proceedings of the 1st Conference of the Extreme Science and Engineeering Discovery Environment: Bridging from the eXtreme to the Campus and Beyond*

James D. "Having it Both Ways: Eclipse PTP on Desktop and Cluster" *Presentation at Scientific Software Days 2012, Austin, TX*

20.9 Metrics

20.9.1 Standard User Assistance Metrics

TACC staff members continue to provide trouble ticket support via the XSEDE ticket system and the TACC Consulting System. 340 tickets, submitted via the XSEDE ticket system, were handled by TACC staff during the report period with 308 being closed. Both trouble ticket systems are monitored 7x24x365 and approximately 25 TACC staff members are engaged in this front-line support activity. The following table indicates the number of tickets opened, closed, and a breakdown of the ticket category.

Issue Category	Number of tickets opened	Number of tickets closed
Jobs/Batch Queues	97	84
Software/Applications	75	68
Login/Access Issues	71	70
System Issues	9	8
Account Issues	32	31
Filesystem Issues	18	17
Other	38	30

TACC ticket resolution times by category from the XSEDE Ticket System

Time to Resolution	account issues	file systems	grid software	jobs/batch queues	login/access issues	mss/data issues	network issues	software/apps	system issues	other
0-1 hr	3			1	2					2
1-24 hr	9	5	1	10	19	4		8	2	1
1-7 d	4	2		11	8	2		8	2	1
1-2 wk	4	2	1	14	3			9	3	2
> 2 wk	4	3		28	6	4	1	24	3	2
Still Open		3		10	2			23	1	4

XSEDE users also may submit requests for assistance via the TACC User Portal (TUP). During the reporting period 192 tickets were submitted through the TUP; 162 have been resolved, 21 are pending user response, and 9 are in progress.

20.9.2 SP-specific Metrics

Allocation usage in section 1.9.3 reflects utilization of TACC resources by the XSEDE user community. There are allocation pools on TACC resources for the non-XSEDE community; the following table indicates the breakdown of available allocation and usage during the reporting period for both major communities. Allocation and usage information is reported in system units (SUs) with an SU being a core hour.

XSEDE/UT Quarter Usage

System	SUs Available	XSEDE SUs Delivered	XSEDE Usage (%)	UT SUs Delivered	UT Usage (%)	Total SUs Delivered
Ranger	138,326,784	116,460,098	92.40	9,576,376	7.60	126,036,474
Lonestar	50,413,160	12,211,277	27	32,389,305	73	44,600,582
Longhorn	4,493,312	1,412,592	57	1,068,928	43	2,481,520
Spur	281,152	8,575	78	2,444	22	11,019

The following table contains system availability statistics for the reporting period for TACC compute, visualization, and storage resources.

TACC Resource Availability Statistics

	Lonestar					Spur				
	Uptime					Uptime				
	PM		Outage			PM		Outage		
Month	#	Hrs	#	Hrs	%Up	#	Hrs	#	Hrs	%Up
2012-10	2	27.50	0	0.00	96.3	0	0.00	0	0.00	100.0
2012-11	0	0.00	0	0.00	100.0	1	11.50	0	0.00	98.4

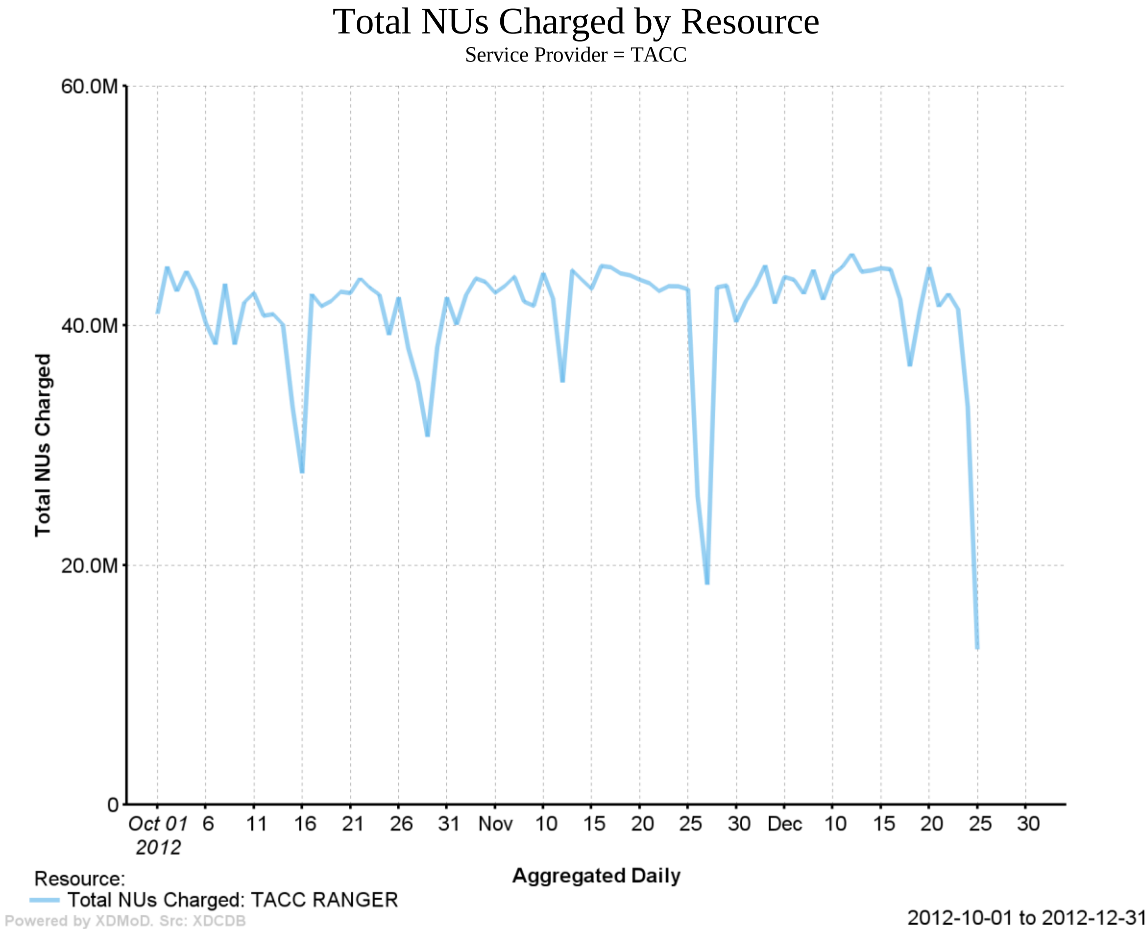
2012-12	0	0.00	0	0.00	100.0	0	0.00	0	0.00	100.0

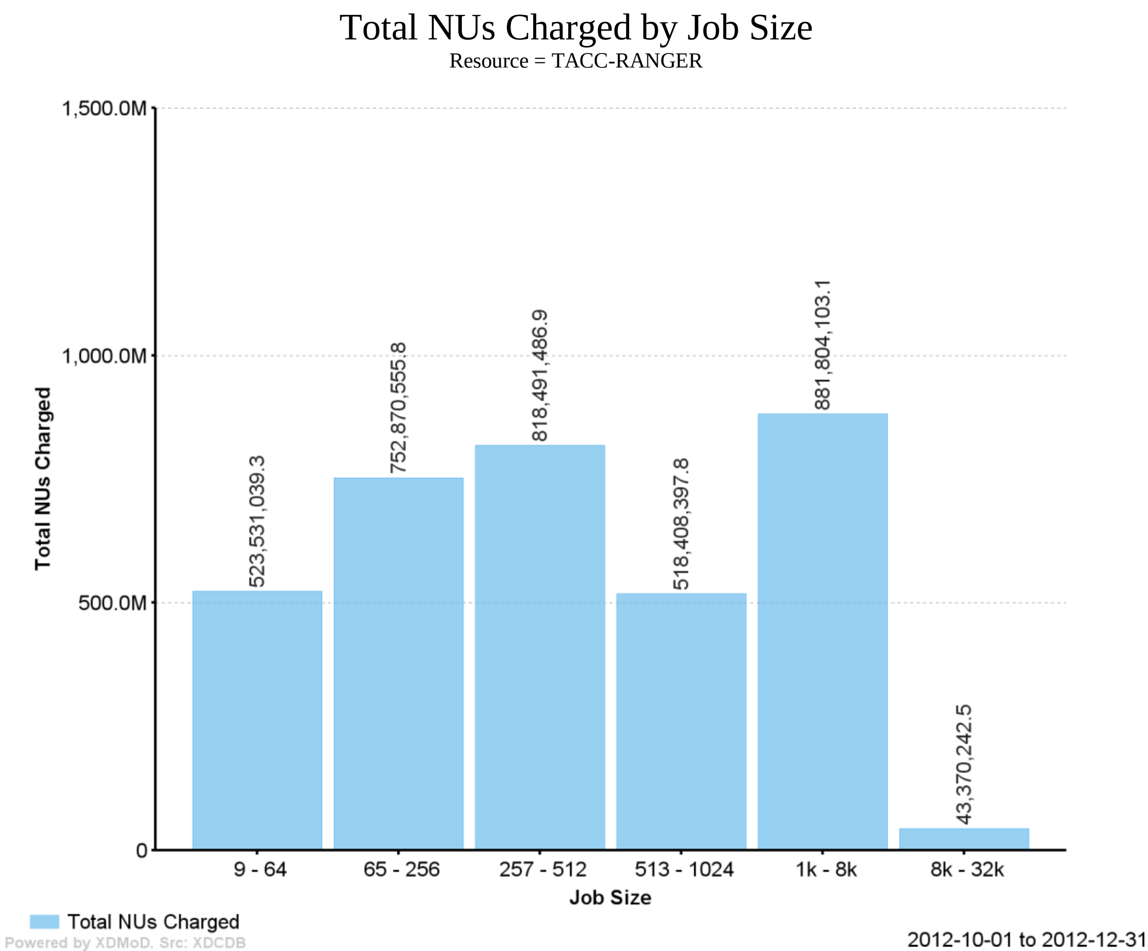
	Ranger					Ranch				
	Uptime					Uptime				
	PM		Outage			PM		Outage		
Month	#	Hrs	#	Hrs	%Up	#	Hrs	#	Hrs	%Up
2012-10	0	0.00	0	0.00	100.0	2	41.00	0	0.00	94.5
2012-11	1	11.50	0	0.00	98.4	0	0.00	0	0.00	100.0
2012-12	0	0.00	0	0.00	100.0	0	0.00	1	1.50	99.8

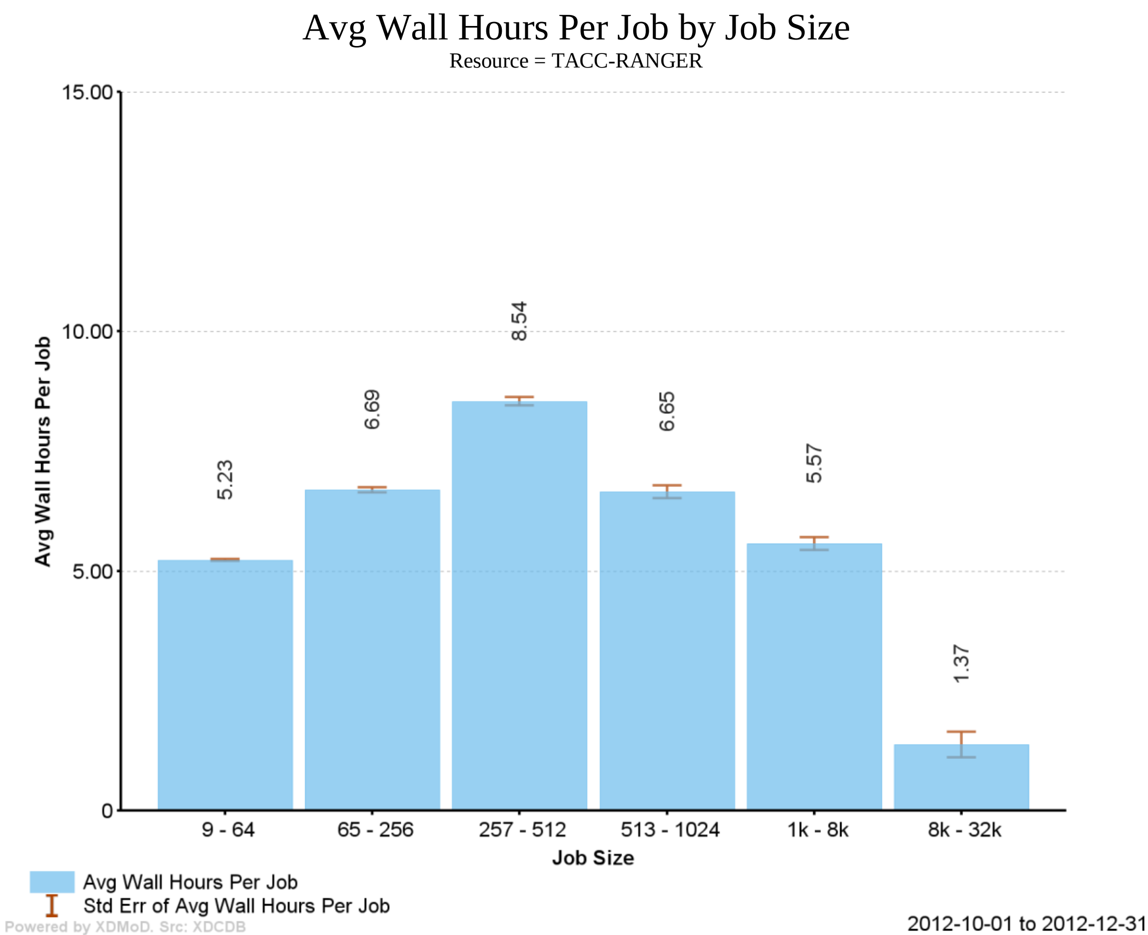
	Longhorn				
	Uptime				
	PM		Outage		
Month	#	Hrs	#	Hrs	%Up
2012-10	1	14.00	0	0.00	98.1
2012-11	0	0.00	0	0.00	100.0
2012-12	0	0.00	0	0.00	100.0

20.9.3 Standard systems metrics

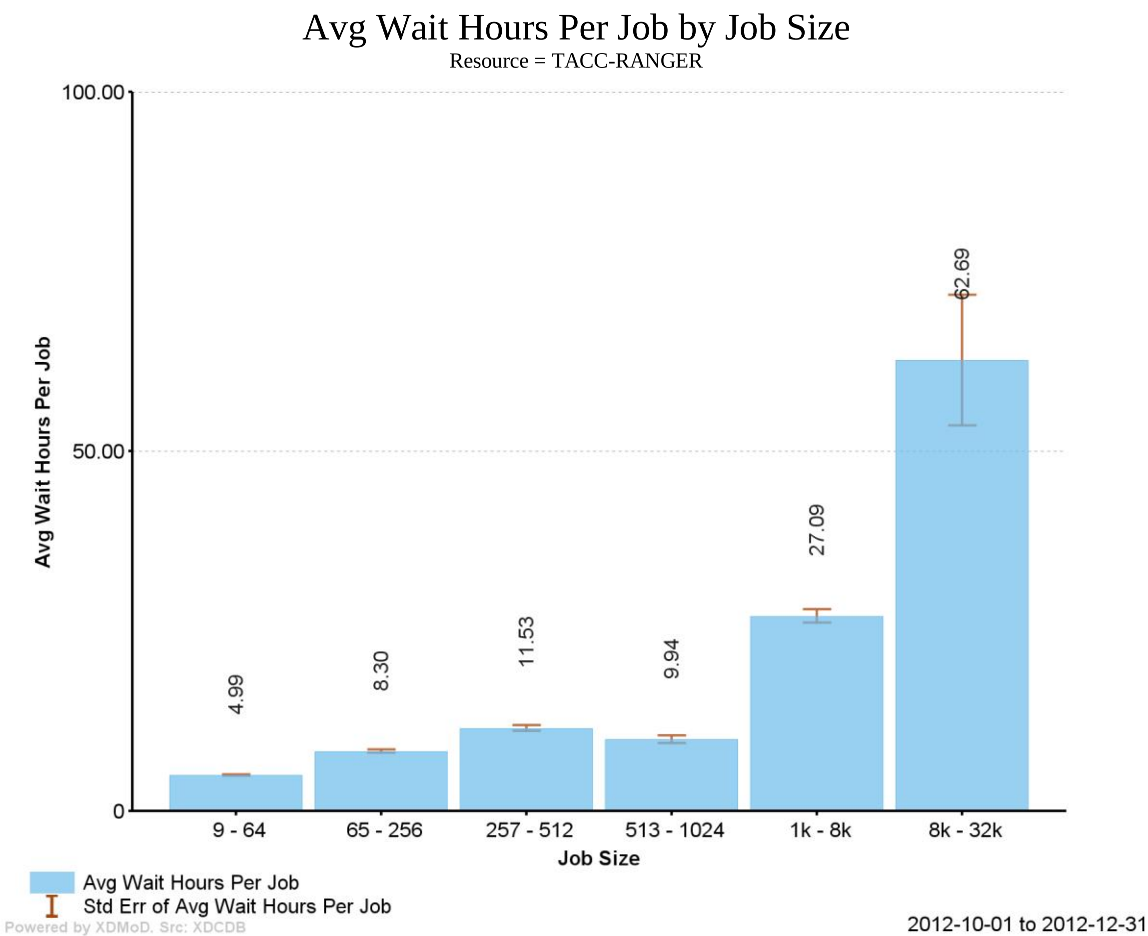
TACC-RANGER Quarterly Report

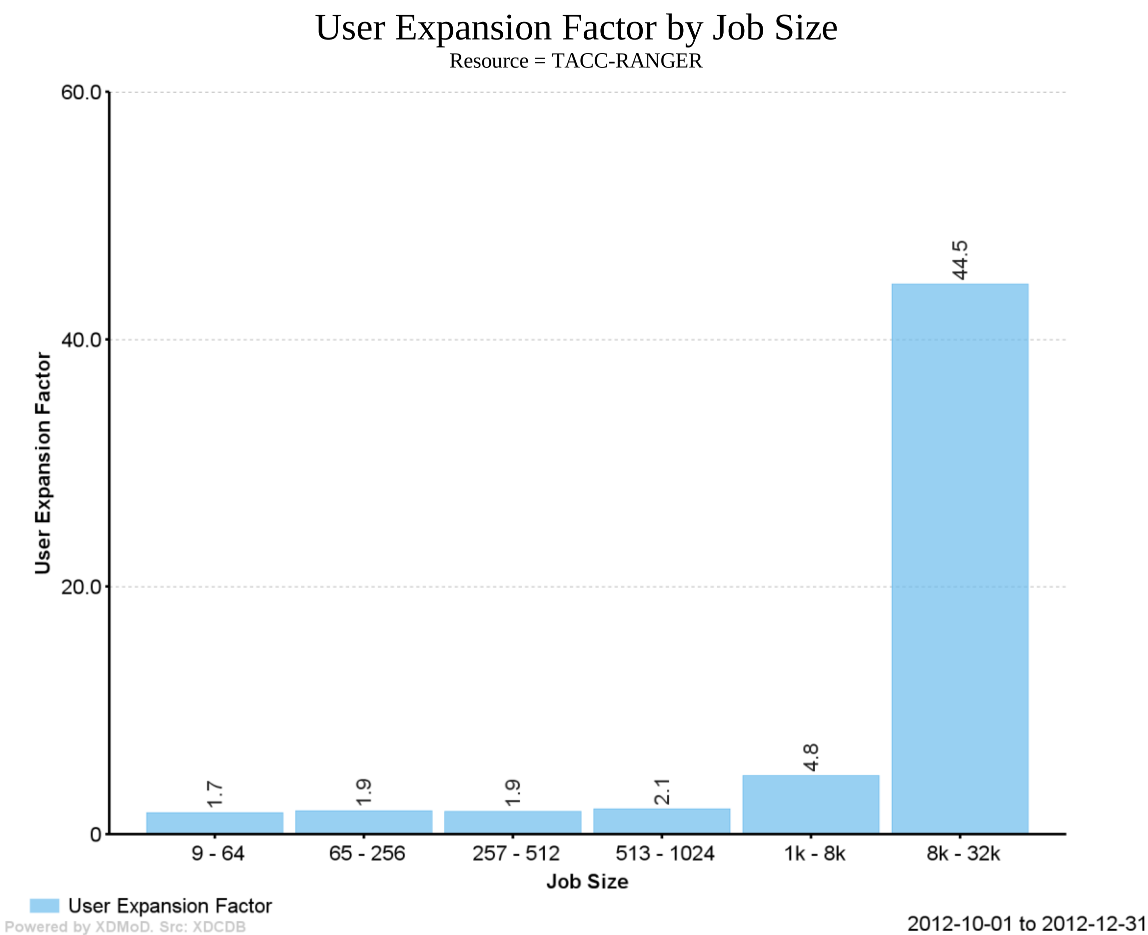


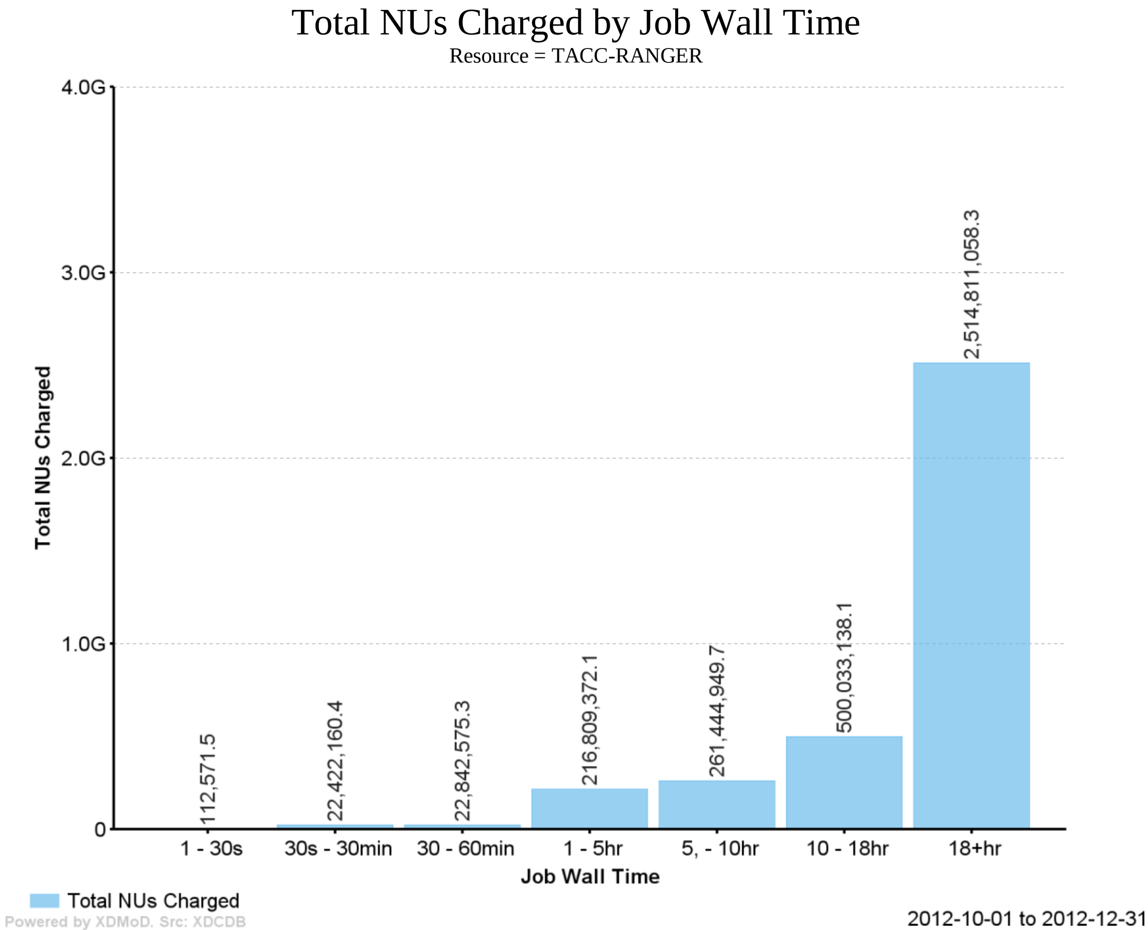

Total NUs Charged by Job Size
Resource = TACC-RANGER
1,500.0M
1,000.0M
500.0M
0
Total NUs Charged
523,531,039.3
752,870,555.8
818,491,486.9
518,408,397.8
881,804,103.1
43,370,242.5
9 - 64
65 - 256
257 - 512
513 - 1024
1k - 8k
8k - 32k
Job Size
Total NUs Charged
Powered by XDMoD. Src: XDCDB
2012-10-01 to 2012-12-31

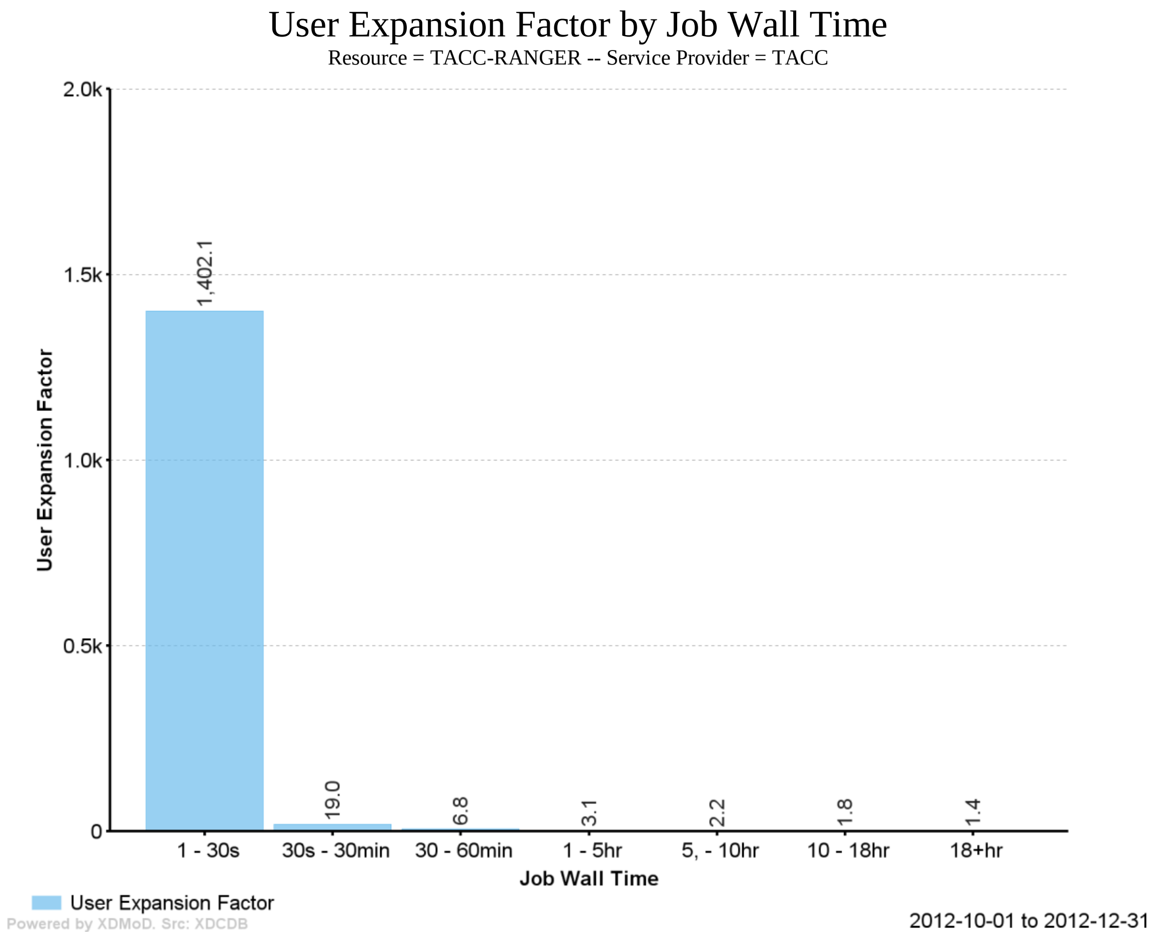


Avg Wall Hours Per Job by Job Size
Resource = TACC-RANGER
15.00
10.00
5.00
0
Avg Wall Hours Per Job
5.23
6.69
8.54
6.65
5.57
1.37
9 - 64
65 - 256
257 - 512
513 - 1024
1k - 8k
8k - 32k
Job Size
Avg Wall Hours Per Job
Std Err of Avg Wall Hours Per Job
Powered by XDMoD. Src: XDCDB
2012-10-01 to 2012-12-31

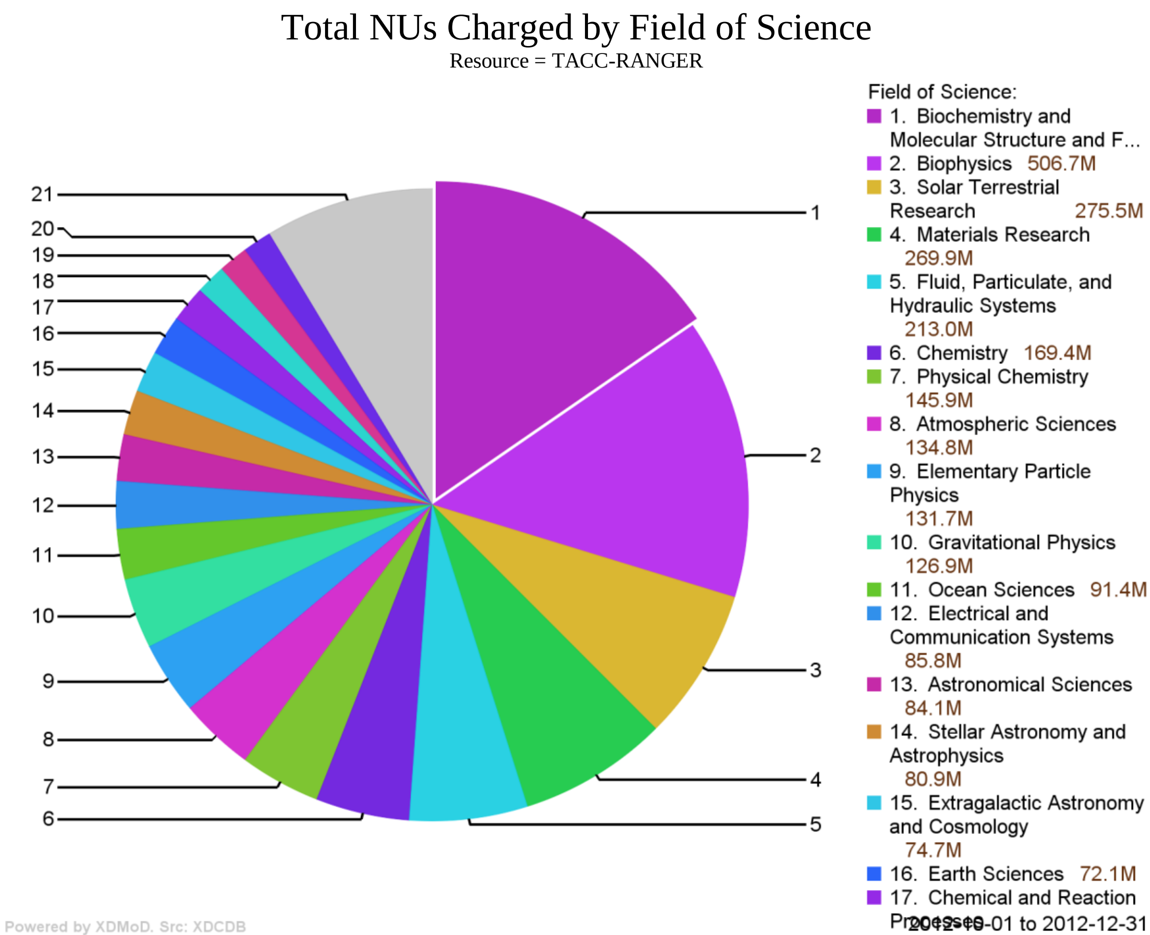

Avg Wait Hours Per Job by Job Size
Resource = TACC-RANGER
100.00
50.00
0
Avg Wait Hours Per Job
4.99
8.30
11.53
9.94
27.09
62.69
9 - 64
65 - 256
257 - 512
513 - 1024
1k - 8k
8k - 32k
Job Size
Avg Wait Hours Per Job
Std Err of Avg Wait Hours Per Job
Powered by XDMoD. Src: XDCDB
2012-10-01 to 2012-12-31


User Expansion Factor by Job Size
Resource = TACC-RANGER
User Expansion Factor
60.0
40.0
20.0
0
44.5
1.7
1.9
1.9
2.1
4.8
9 - 64
65 - 256
257 - 512
513 - 1024
1k - 8k
8k - 32k
Job Size
User Expansion Factor
Powered by XDMoD. Src: XDCDB
2012-10-01 to 2012-12-31


Total NUs Charged by Job Wall Time
Resource = TACC-RANGER
4.0G
3.0G
2.0G
1.0G
0
Total NUs Charged
112,571.5
22,422,160.4
22,842,575.3
216,809,372.1
261,444,949.7
500,033,138.1
2,514,811,058.3
1 - 30s
30s - 30min
30 - 60min
1 - 5hr
5, - 10hr
10 - 18hr
18+hr
Job Wall Time
Total NUs Charged
Powered by XDMoD. Src: XDCDB
2012-10-01 to 2012-12-31

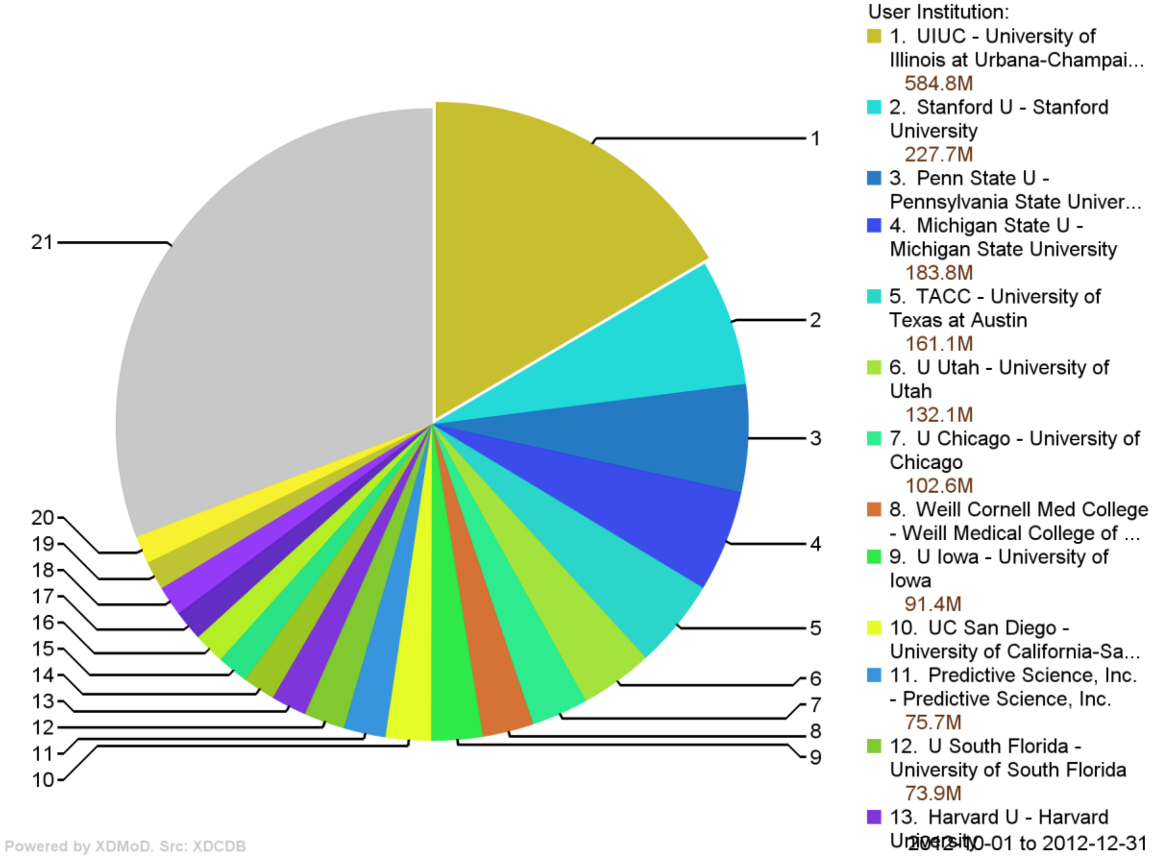


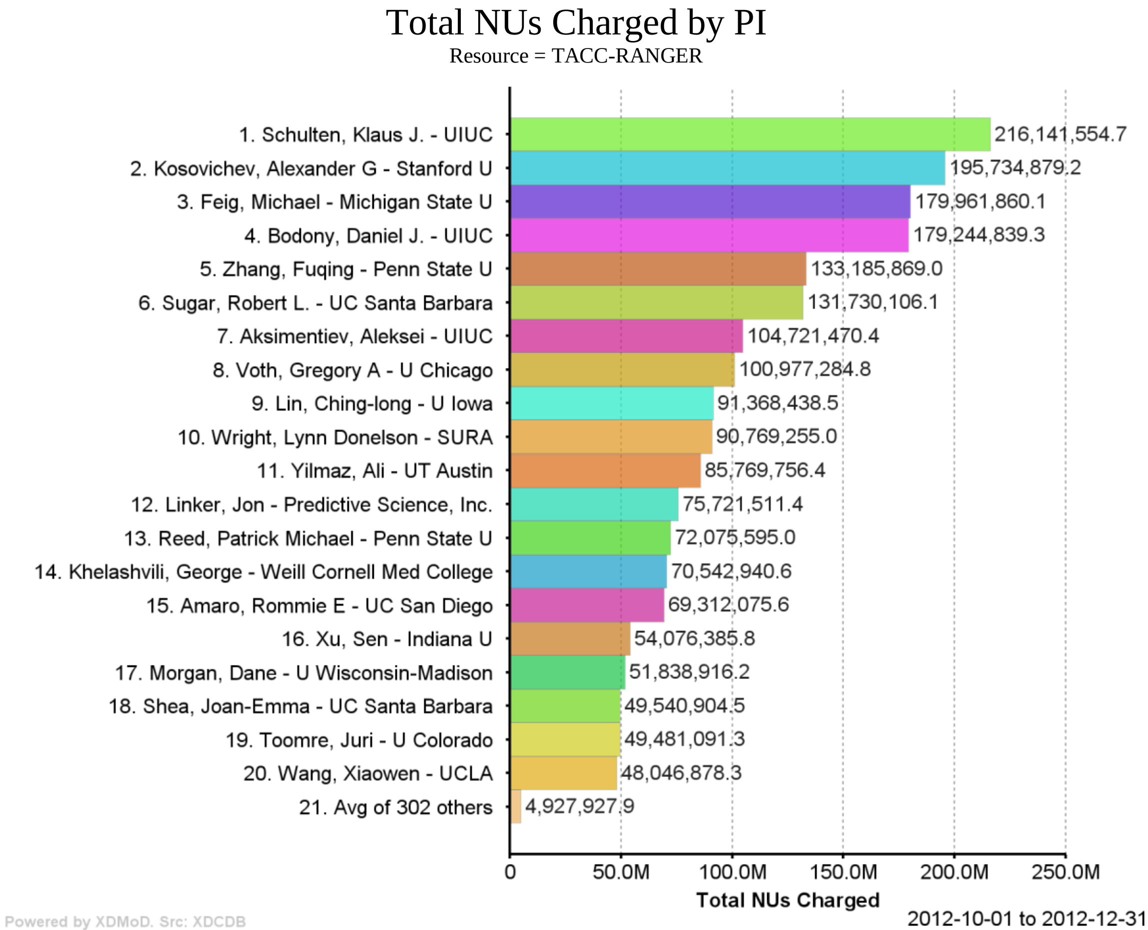
User Expansion Factor by Job Wall Time
Resource = TACC-RANGER -- Service Provider = TACC
2.0k
1.5k
1.0k
0.5k
0
User Expansion Factor
1,402.1
19.0
6.8
3.1
2.2
1.8
1.4
1 - 30s
30s - 30min
30 - 60min
1 - 5hr
5, - 10hr
10 - 18hr
18+hr
Job Wall Time
User Expansion Factor
Powered by XDMoD. Src: XDCDB
2012-10-01 to 2012-12-31


Total NUs Charged by Field of Science
Resource = TACC-RANGER
Field of Science:
1. Biochemistry and Molecular Structure and F...
2. Biophysics 506.7M
3. Solar Terrestrial Research 275.5M
4. Materials Research 269.9M
5. Fluid, Particulate, and Hydraulic Systems 213.0M
6. Chemistry 169.4M
7. Physical Chemistry 145.9M
8. Atmospheric Sciences 134.8M
9. Elementary Particle Physics 131.7M
10. Gravitational Physics 126.9M
11. Ocean Sciences 91.4M
12. Electrical and Communication Systems 85.8M
13. Astronomical Sciences 84.1M
14. Stellar Astronomy and Astrophysics 80.9M
15. Extragalactic Astronomy and Cosmology 74.7M
16. Earth Sciences 72.1M
17. Chemical and Reaction Processes
2012-10-01 to 2012-12-31
Powered by XDMoD. Src: XDCDB

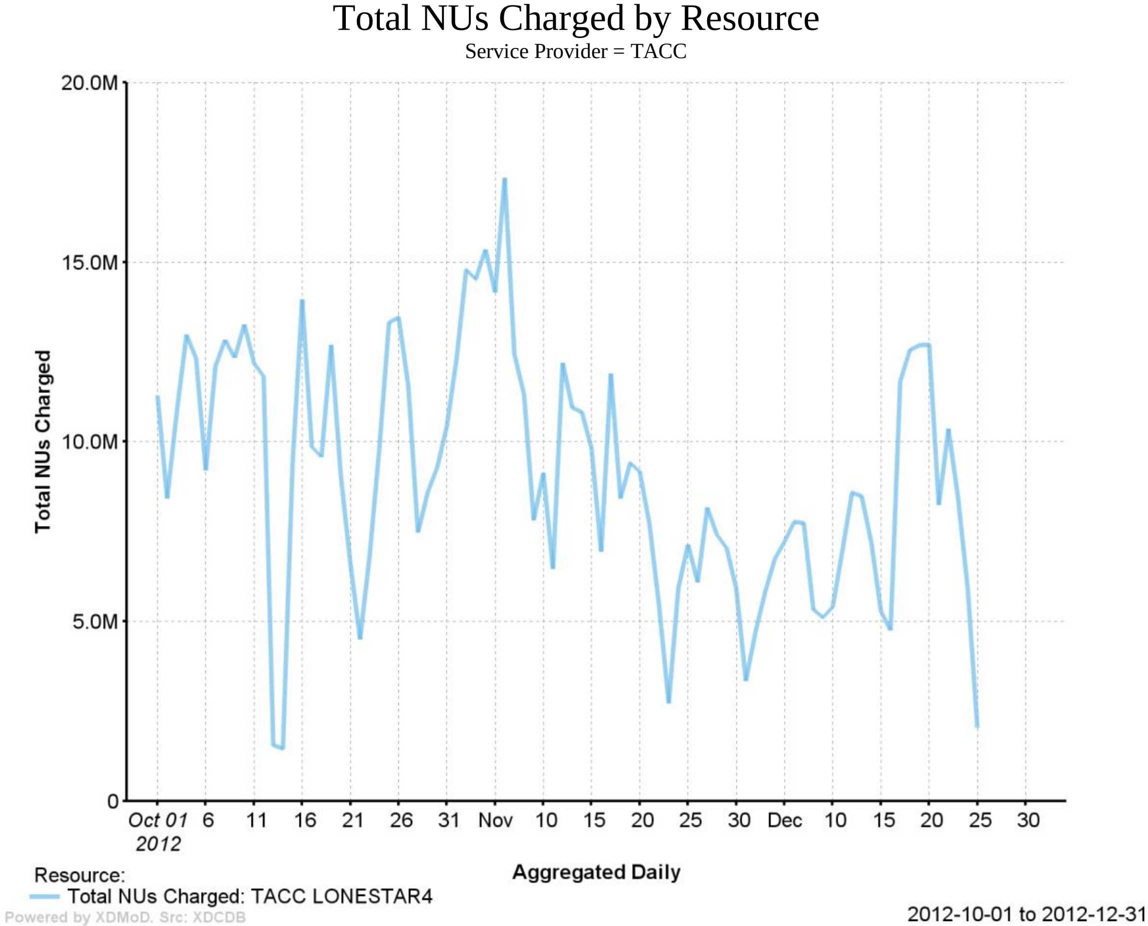
Total NUs Charged by User Institution

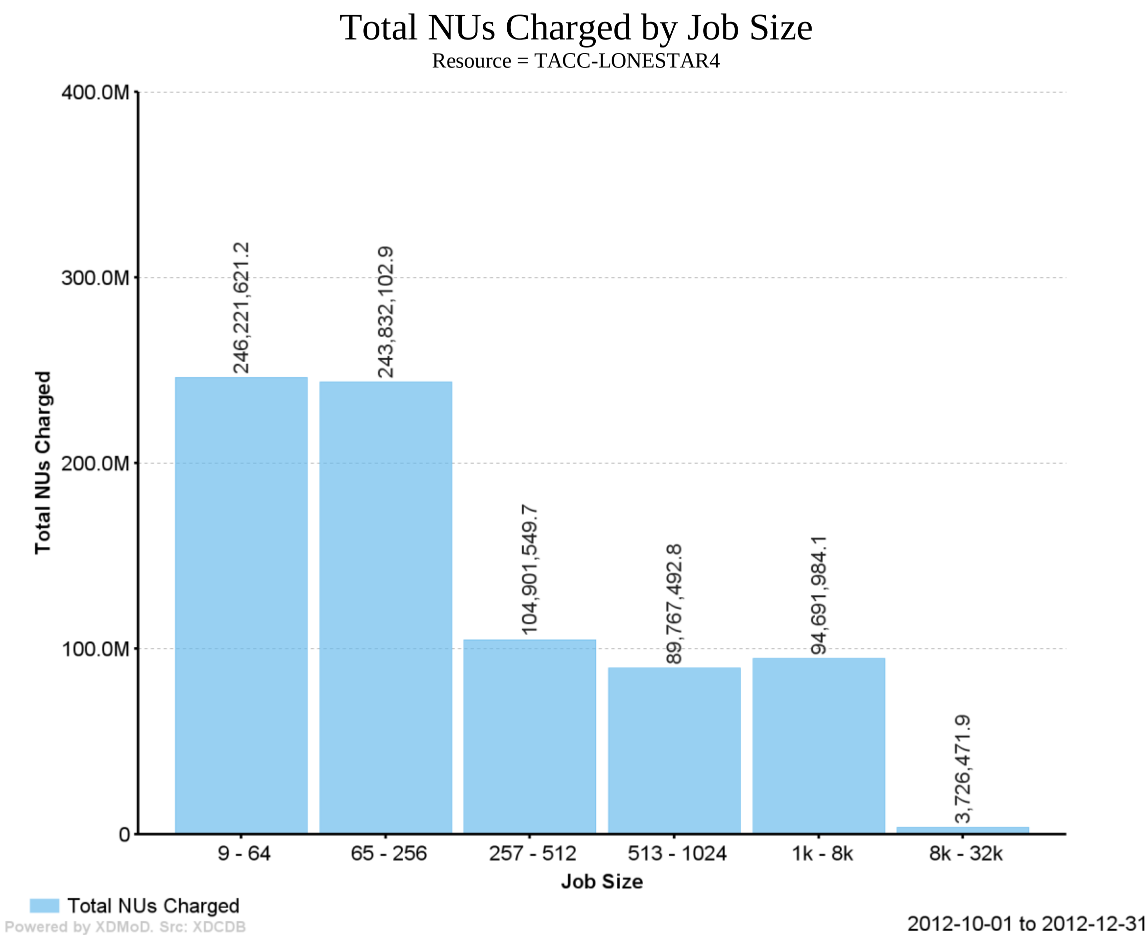
Resource = TACC-RANGER

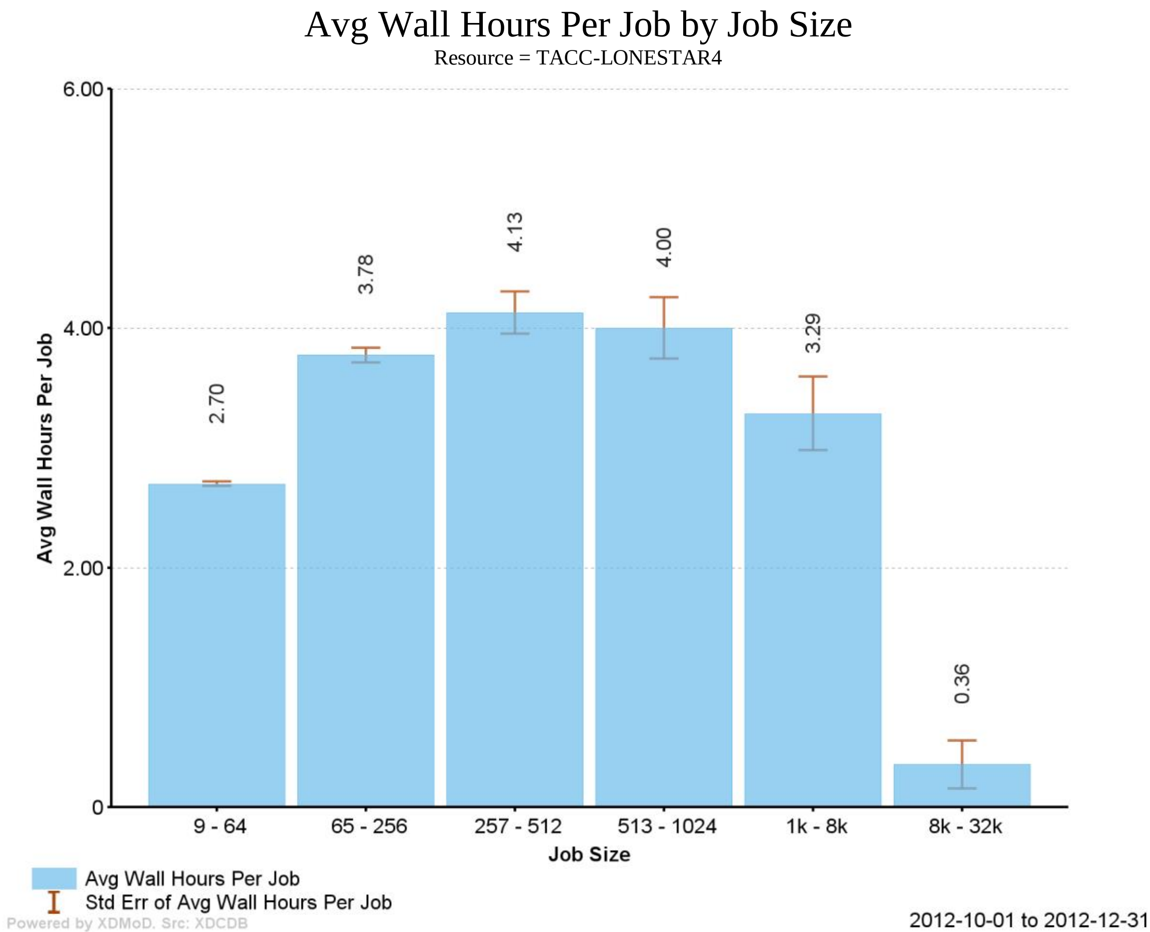


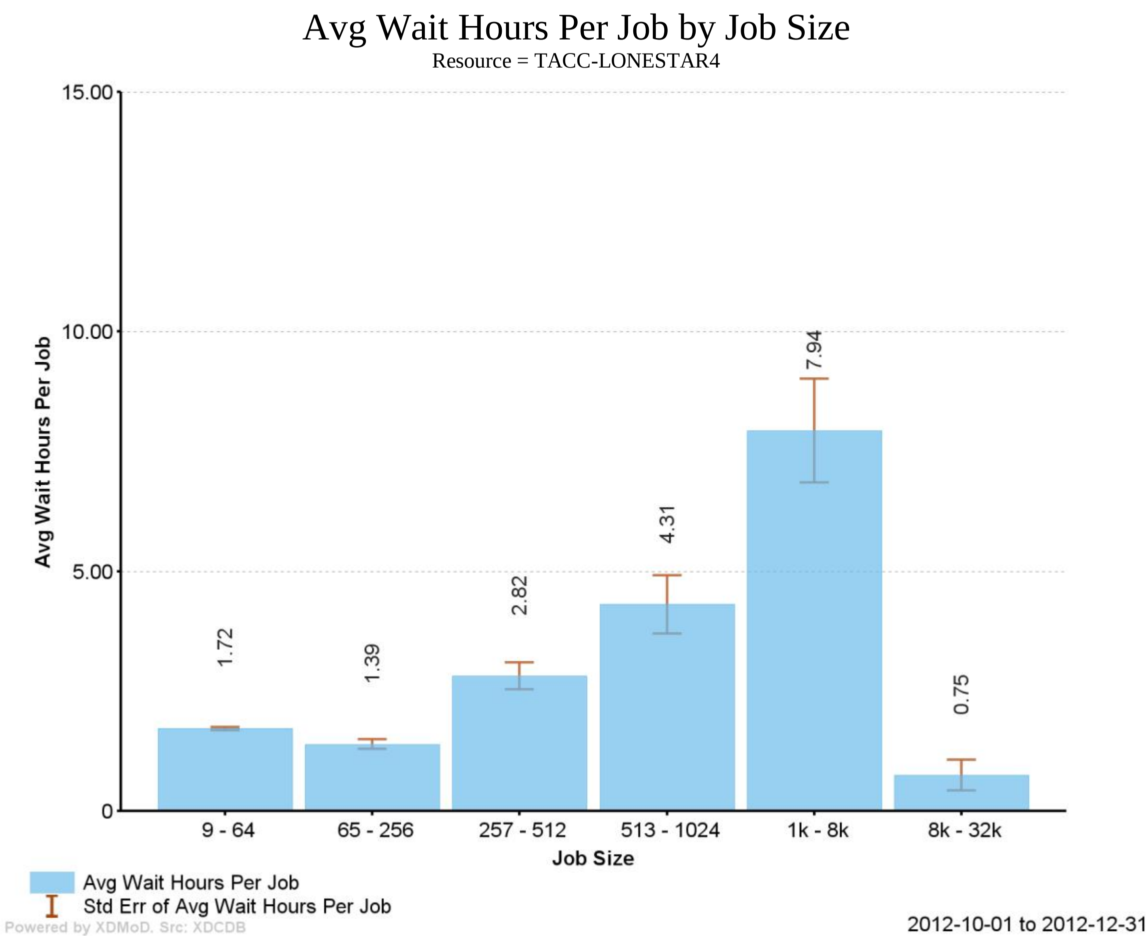

Total NUs Charged by PI
Resource = TACC-RANGER
1. Schulten, Klaus J. - UIUC
2. Kosovichev, Alexander G - Stanford U
3. Feig, Michael - Michigan State U
4. Bodony, Daniel J. - UIUC
5. Zhang, Fuqing - Penn State U
6. Sugar, Robert L. - UC Santa Barbara
7. Aksimentiev, Aleksei - UIUC
8. Voth, Gregory A - U Chicago
9. Lin, Ching-long - U Iowa
10. Wright, Lynn Donelson - SURA
11. Yilmaz, Ali - UT Austin
12. Linker, Jon - Predictive Science, Inc.
13. Reed, Patrick Michael - Penn State U
14. Khelashvili, George - Weill Cornell Med College
15. Amaro, Rommie E - UC San Diego
16. Xu, Sen - Indiana U
17. Morgan, Dane - U Wisconsin-Madison
18. Shea, Joan-Emma - UC Santa Barbara
19. Toomre, Juri - U Colorado
20. Wang, Xiaowen - UCLA
21. Avg of 302 others
216,141,554.7
195,734,879.2
179,961,860.1
179,244,839.3
133,185,869.0
131,730,106.1
104,721,470.4
100,977,284.8
91,368,438.5
90,769,255.0
85,769,756.4
75,721,511.4
72,075,595.0
70,542,940.6
69,312,075.6
54,076,385.8
51,838,916.2
49,540,904.5
49,481,091.3
48,046,878.3
4,927,927.9
0
50.0M
100.0M
150.0M
200.0M
250.0M
Total NUs Charged
Powered by XDMoD. Src: XDCDB
2012-10-01 to 2012-12-31

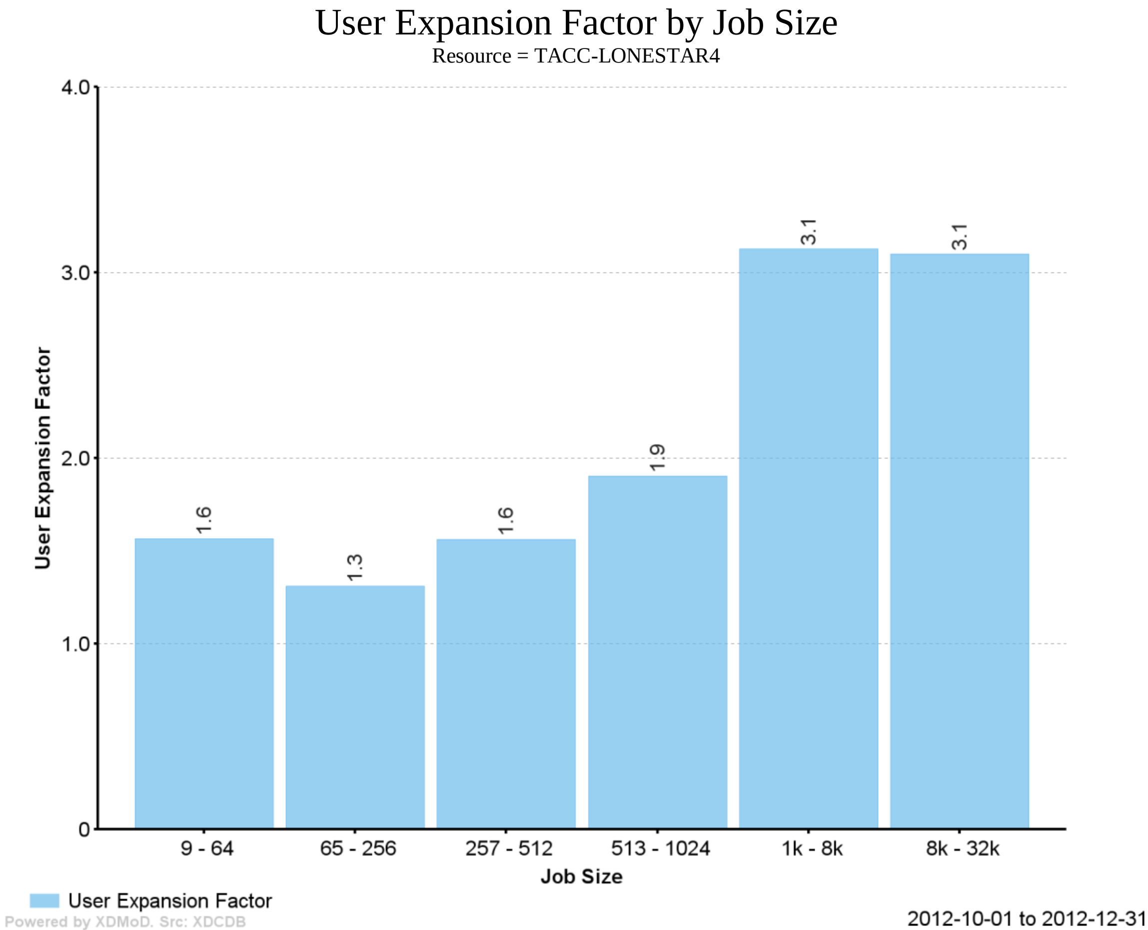
TACC-LONESTAR4 Quarterly Report

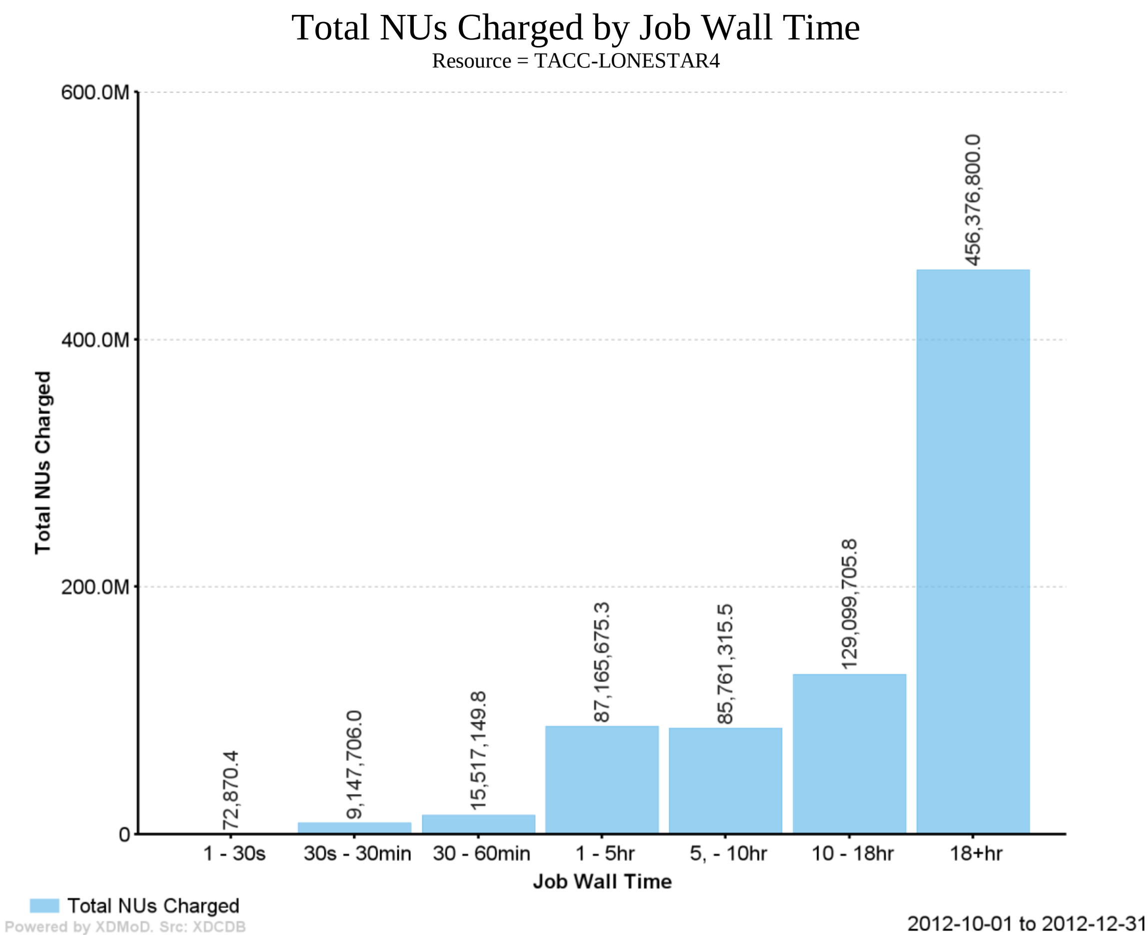



Total NUs Charged by Job Size
Resource = TACC-LONESTAR4
400.0M
300.0M
200.0M
100.0M
0
Total NUs Charged
246,221,621.2
243,832,102.9
104,901,549.7
89,767,492.8
94,691,984.1
3,726,471.9
9 - 64
65 - 256
257 - 512
513 - 1024
1k - 8k
8k - 32k
Job Size
Total NUs Charged
Powered by XDMoD. Src: XDCDB
2012-10-01 to 2012-12-31

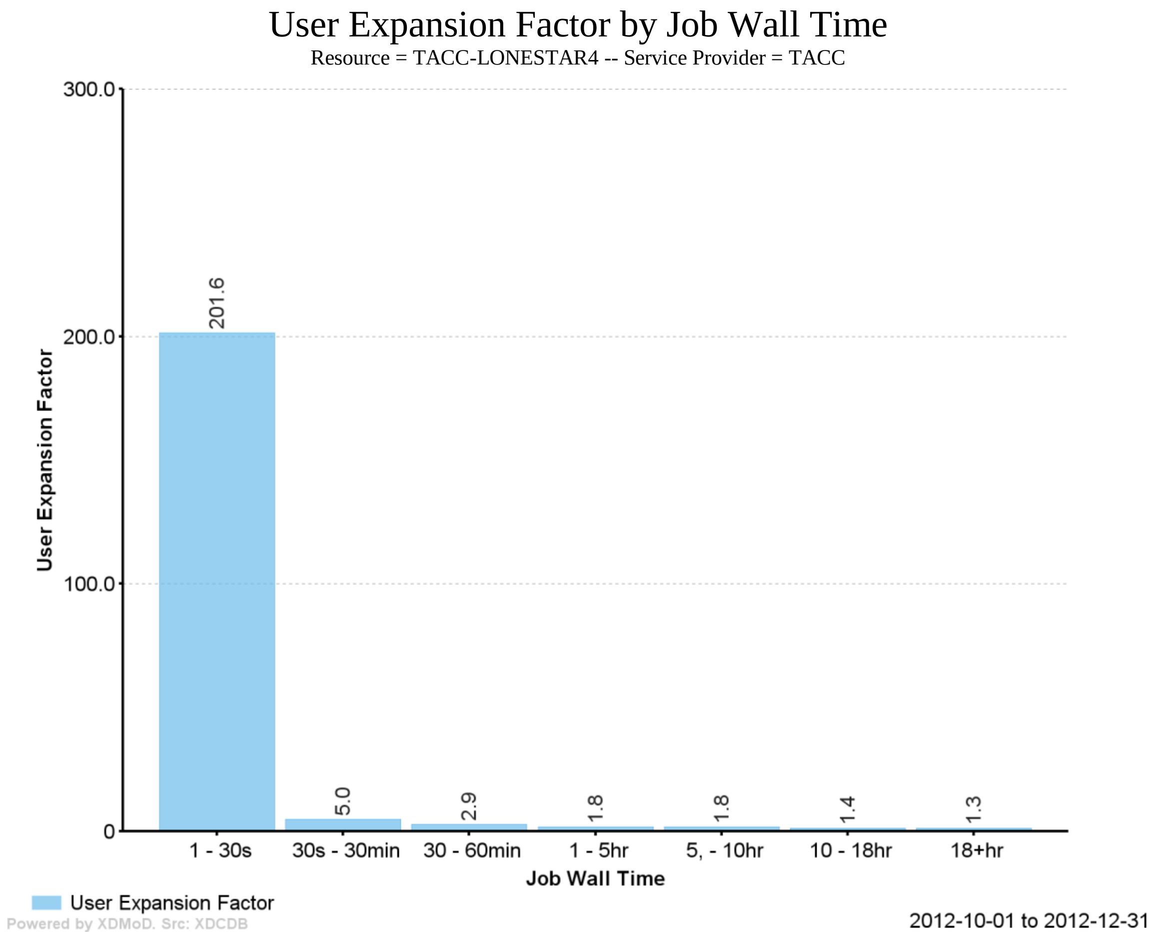

Avg Wall Hours Per Job by Job Size
Resource = TACC-LONESTAR4
6.00
4.00
2.00
0
Avg Wall Hours Per Job
2.70
3.78
4.13
4.00
3.29
0.36
9 - 64
65 - 256
257 - 512
513 - 1024
1k - 8k
8k - 32k
Job Size
Avg Wall Hours Per Job
Std Err of Avg Wall Hours Per Job
Powered by XDMoD. Src: XDCDB
2012-10-01 to 2012-12-31


Avg Wait Hours Per Job by Job Size
Resource = TACC-LONESTAR4
15.00
10.00
5.00
0
Avg Wait Hours Per Job
1.72
1.39
2.82
4.31
7.94
0.75
9 - 64
65 - 256
257 - 512
513 - 1024
1k - 8k
8k - 32k
Job Size
Avg Wait Hours Per Job
Std Err of Avg Wait Hours Per Job
Powered by XDMoD. Src: XDCDB
2012-10-01 to 2012-12-31

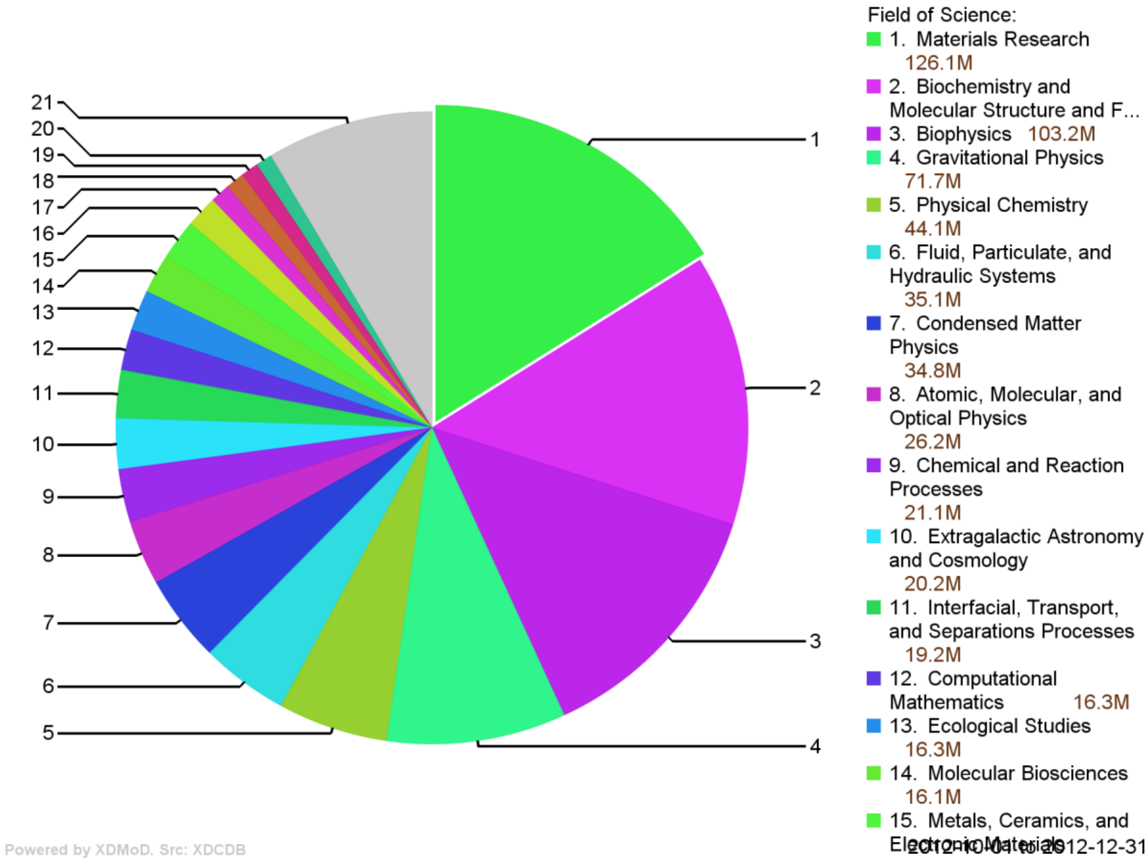

User Expansion Factor by Job Size
Resource = TACC-LONESTAR4
4.0
3.0
2.0
1.0
0
User Expansion Factor
1.6
1.3
1.6
1.9
3.1
3.1
9 - 64
65 - 256
257 - 512
513 - 1024
1k - 8k
8k - 32k
Job Size
User Expansion Factor
Powered by XDMoD. Src: XDCDB
2012-10-01 to 2012-12-31



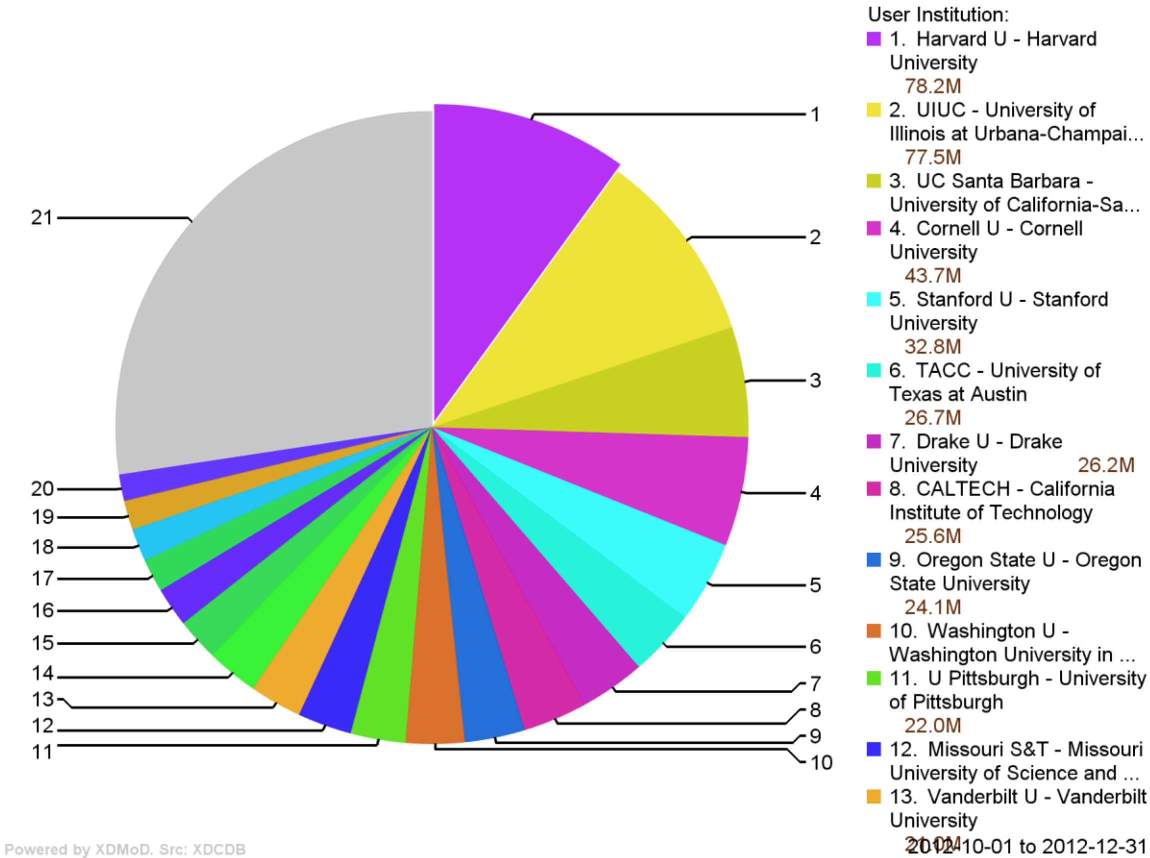
Total NUs Charged by Job Wall Time
Resource = TACC-LONESTAR4
600.0M
400.0M
200.0M
0
Total NUs Charged
72,870.4
9,147,706.0
15,517,149.8
87,165,675.3
85,761,315.5
129,099,705.8
456,376,800.0
1 - 30s
30s - 30min
30 - 60min
1 - 5hr
5, - 10hr
10 - 18hr
18+hr
Job Wall Time
Total NUs Charged
Powered by XDMoD. Src: XDCDB
2012-10-01 to 2012-12-31

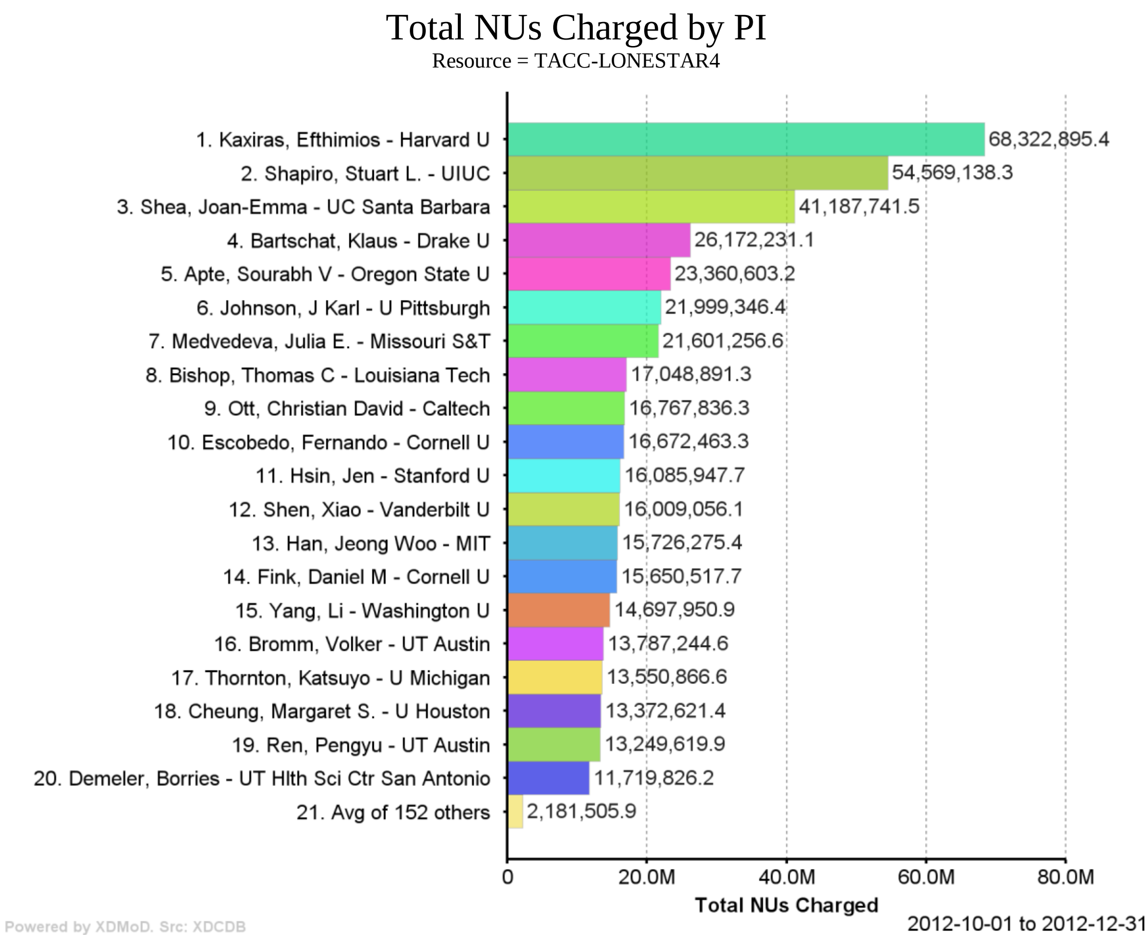

User Expansion Factor by Job Wall Time
Resource = TACC-LONESTAR4 -- Service Provider = TACC
User Expansion Factor
300.0
200.0
100.0
0
201.6
5.0
2.9
1.8
1.8
1.4
1.3
1 - 30s
30s - 30min
30 - 60min
1 - 5hr
5, - 10hr
10 - 18hr
18+hr
Job Wall Time
User Expansion Factor
Powered by XDMoD. Src: XDCDB
2012-10-01 to 2012-12-31

Total NUs Charged by Field of Science
Resource = TACC-LONESTAR4

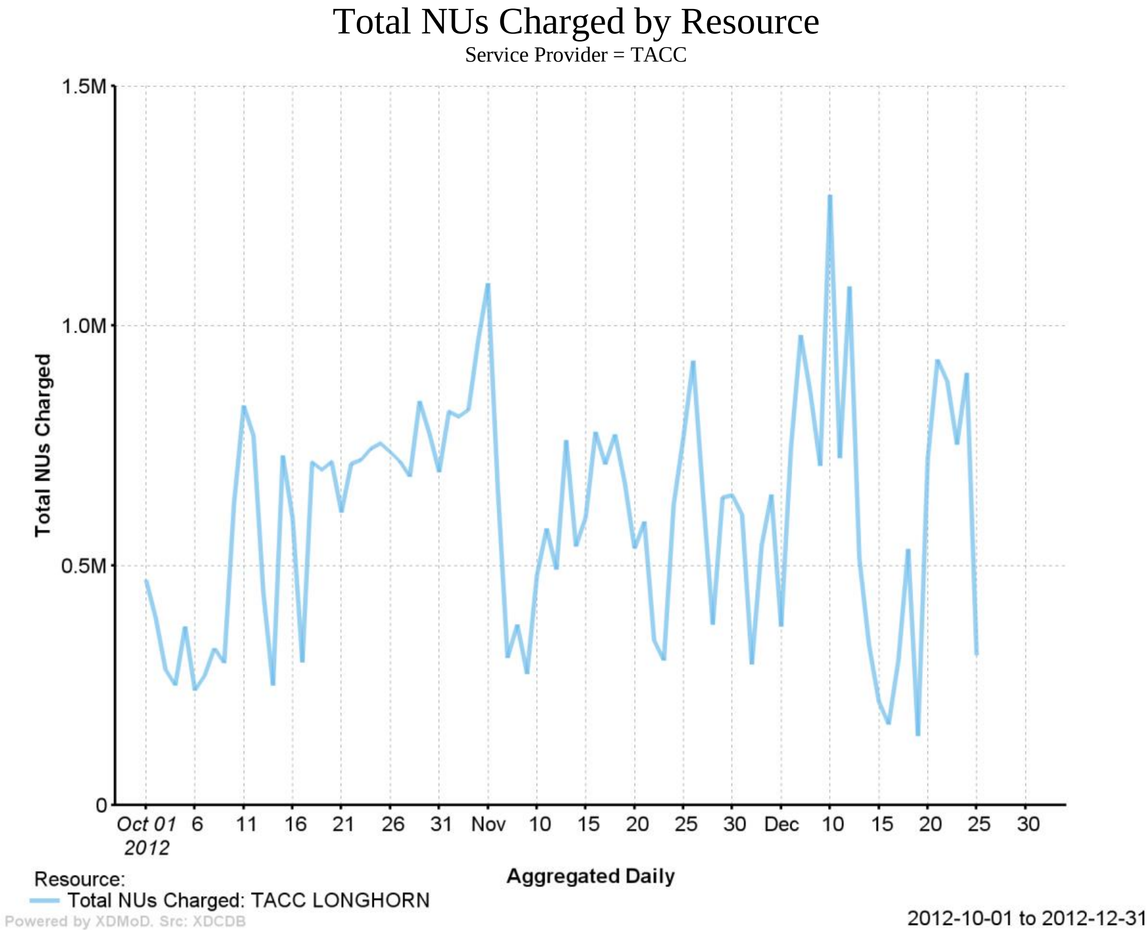


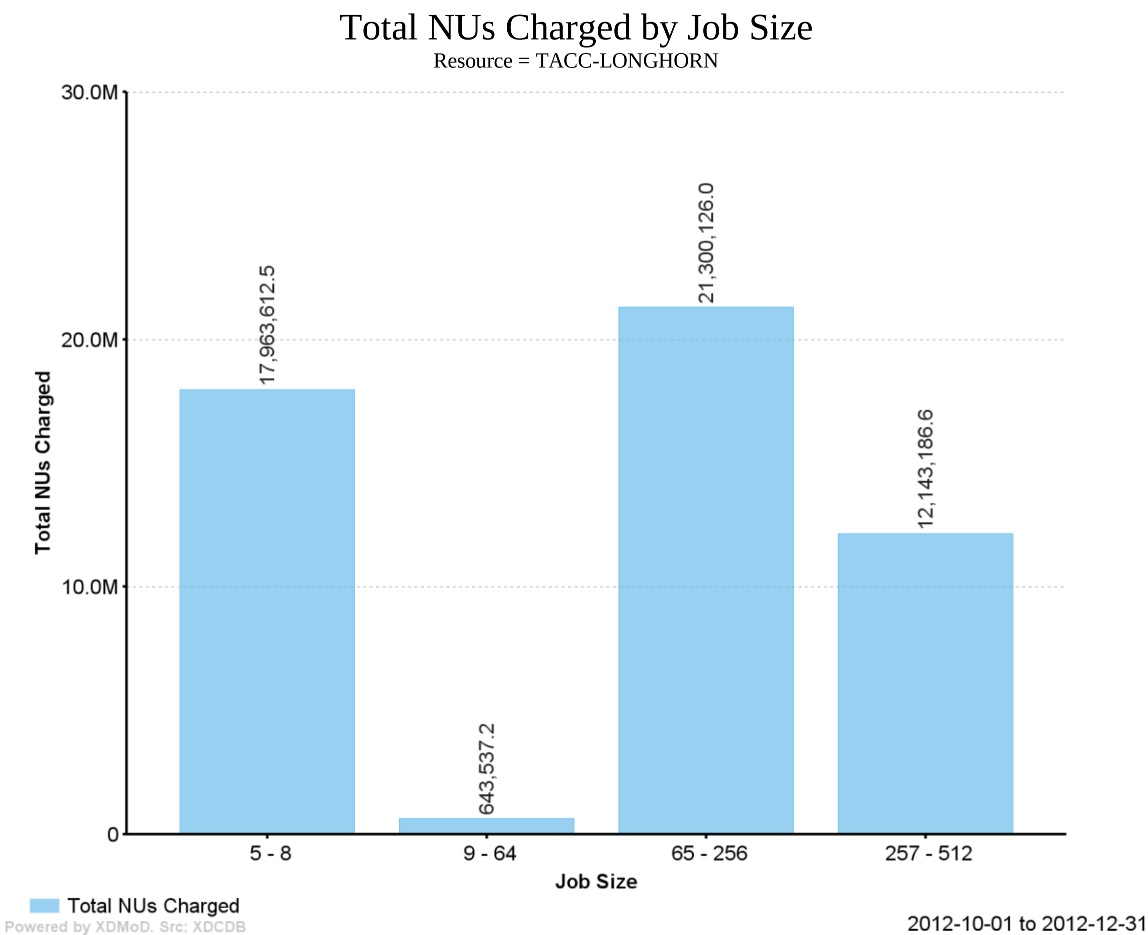
Total NUs Charged by User Institution
Resource = TACC-LONESTAR4




Total NUs Charged by PI
Resource = TACC-LONESTAR4
1. Kaxiras, Efthimios - Harvard U
68,322,895.4
2. Shapiro, Stuart L. - UIUC
54,569,138.3
3. Shea, Joan-Emma - UC Santa Barbara
41,187,741.5
4. Bartschat, Klaus - Drake U
26,172,231.1
5. Apte, Sourabh V - Oregon State U
23,360,603.2
6. Johnson, J Karl - U Pittsburgh
21,999,346.4
7. Medvedeva, Julia E. - Missouri S&T
21,601,256.6
8. Bishop, Thomas C - Louisiana Tech
17,048,891.3
9. Ott, Christian David - Caltech
16,767,836.3
10. Escobedo, Fernando - Cornell U
16,672,463.3
11. Hsin, Jen - Stanford U
16,085,947.7
12. Shen, Xiao - Vanderbilt U
16,009,056.1
13. Han, Jeong Woo - MIT
15,726,275.4
14. Fink, Daniel M - Cornell U
15,650,517.7
15. Yang, Li - Washington U
14,697,950.9
16. Bromm, Volker - UT Austin
13,787,244.6
17. Thornton, Katsuyo - U Michigan
13,550,866.6
18. Cheung, Margaret S. - U Houston
13,372,621.4
19. Ren, Pengyu - UT Austin
13,249,619.9
20. Demeler, Borries - UT Hlth Sci Ctr San Antonio
11,719,826.2
21. Avg of 152 others
2,181,505.9
0
20.0M
40.0M
60.0M
80.0M
Total NUs Charged
2012-10-01 to 2012-12-31
Powered by XDMoD. Src: XDCDB

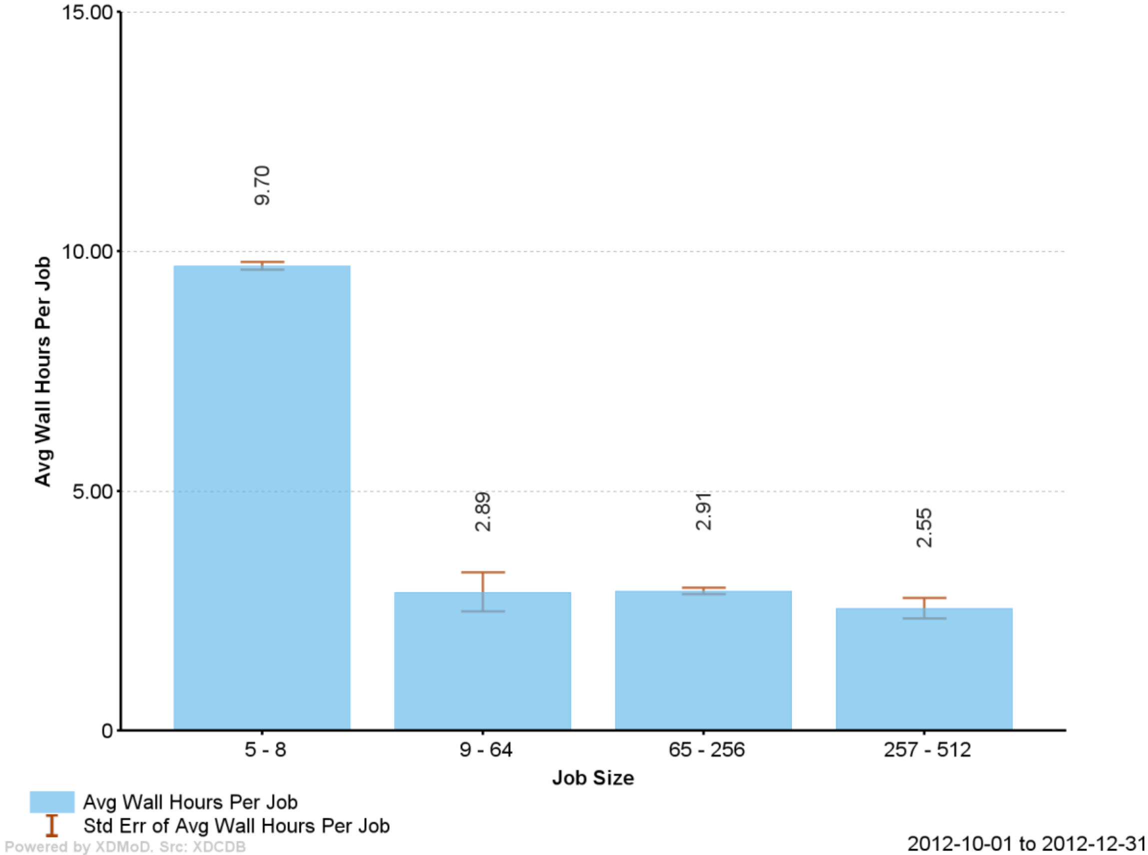
TACC-LONGHORN Quarterly Report

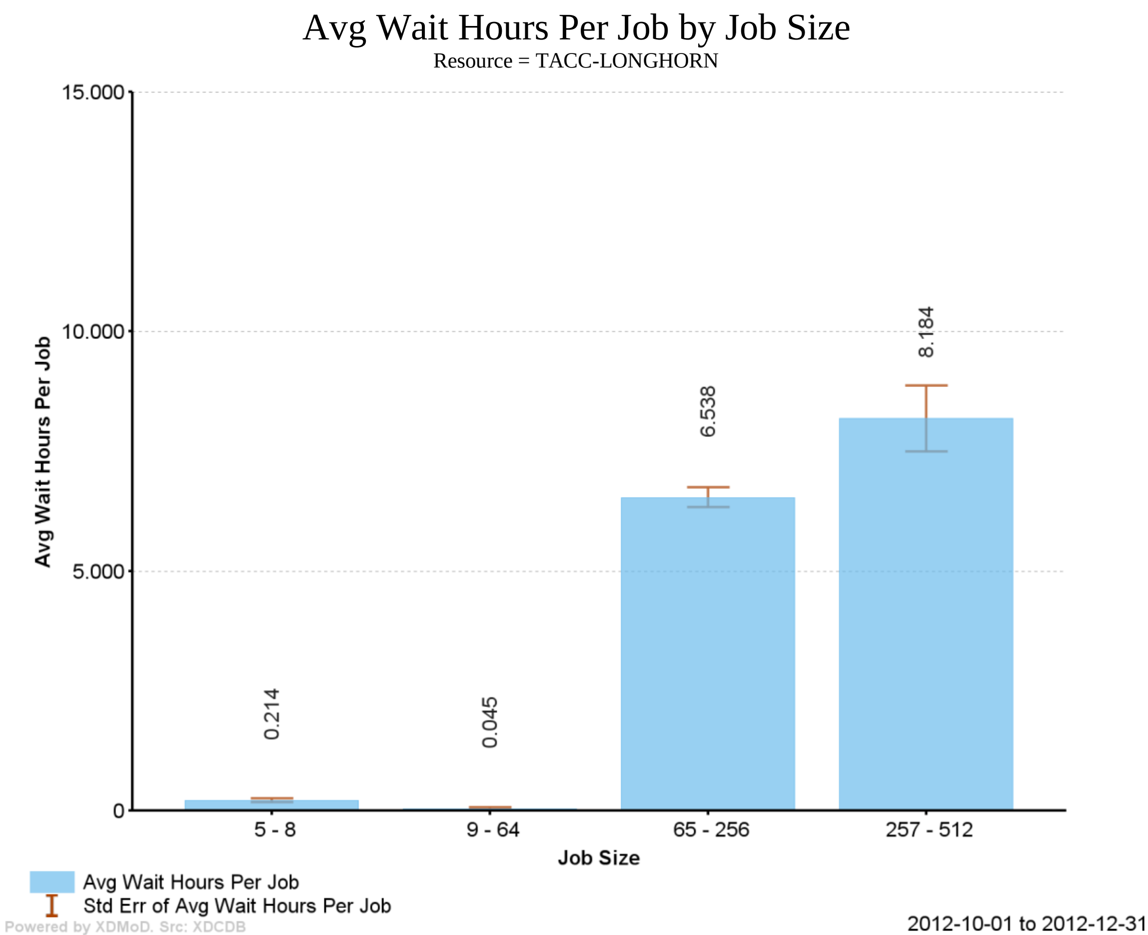



Total NUs Charged by Job Size
Resource = TACC-LONGHORN
30.0M
20.0M
10.0M
0
Total NUs Charged
17,963,612.5
643,537.2
21,300,126.0
12,143,186.6
5 - 8
9 - 64
65 - 256
257 - 512
Job Size
Total NUs Charged
Powered by XDMoD. Src: XDCDB
2012-10-01 to 2012-12-31

Avg Wall Hours Per Job by Job Size

Resource = TACC-LONGHORN

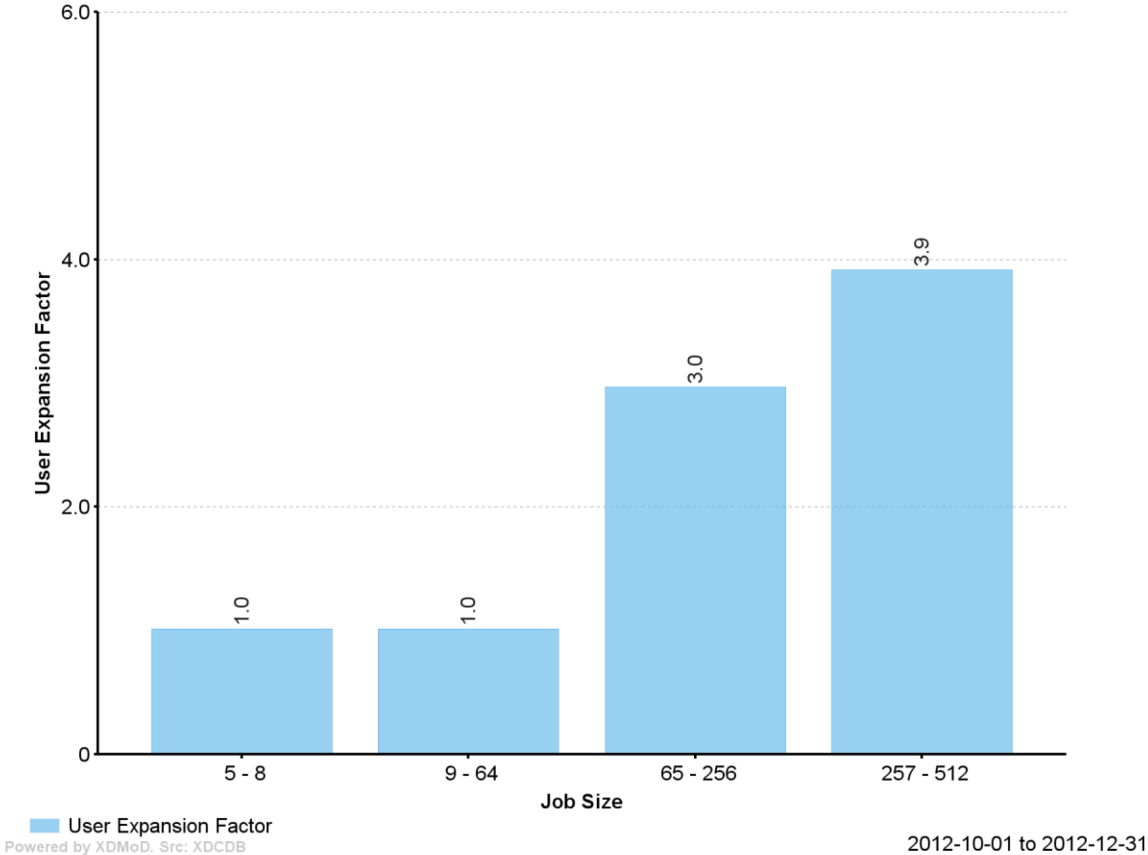


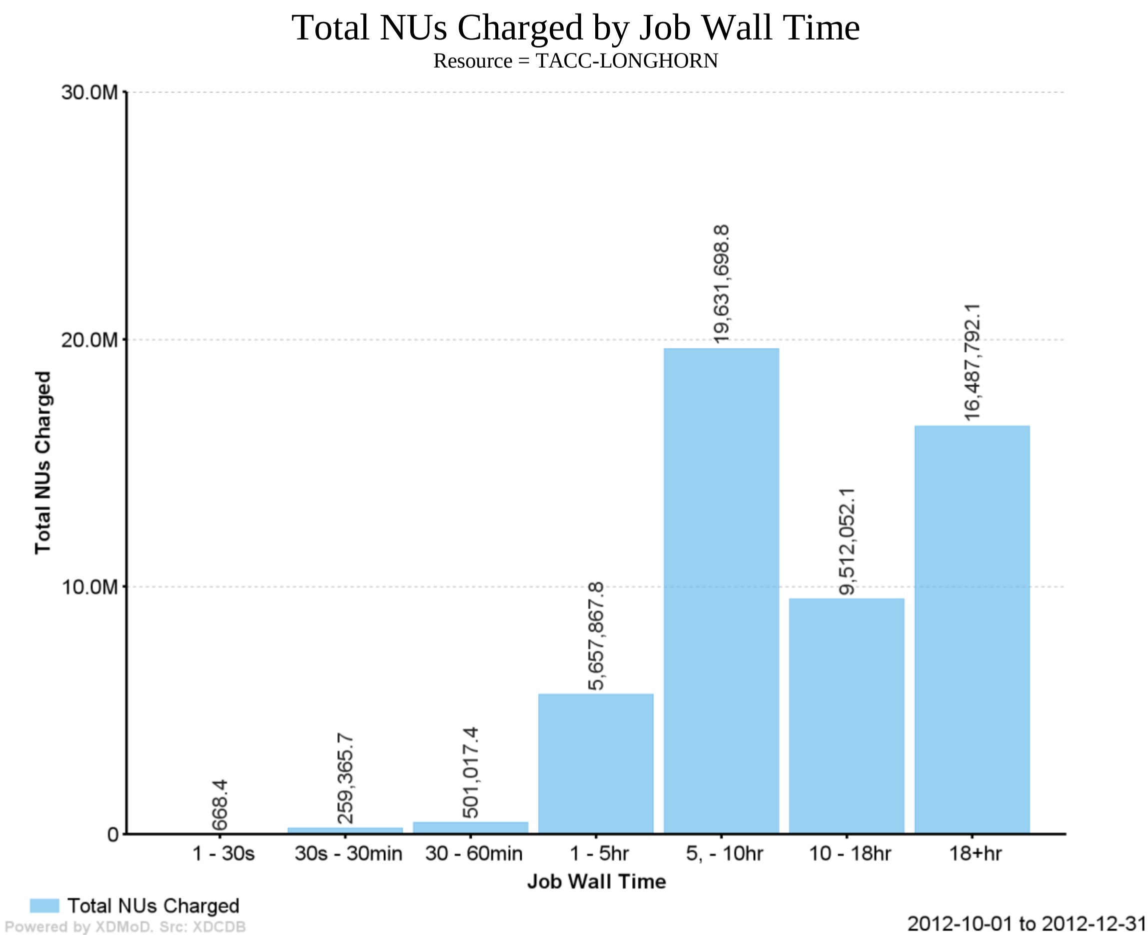


Avg Wait Hours Per Job by Job Size
Resource = TACC-LONGHORN
15.000
10.000
5.000
0
Avg Wait Hours Per Job
0.214
0.045
6.538
8.184
5 - 8
9 - 64
65 - 256
257 - 512
Job Size
Avg Wait Hours Per Job
Std Err of Avg Wait Hours Per Job
Powered by XDMoD. Src: XDCDB
2012-10-01 to 2012-12-31

User Expansion Factor by Job Size

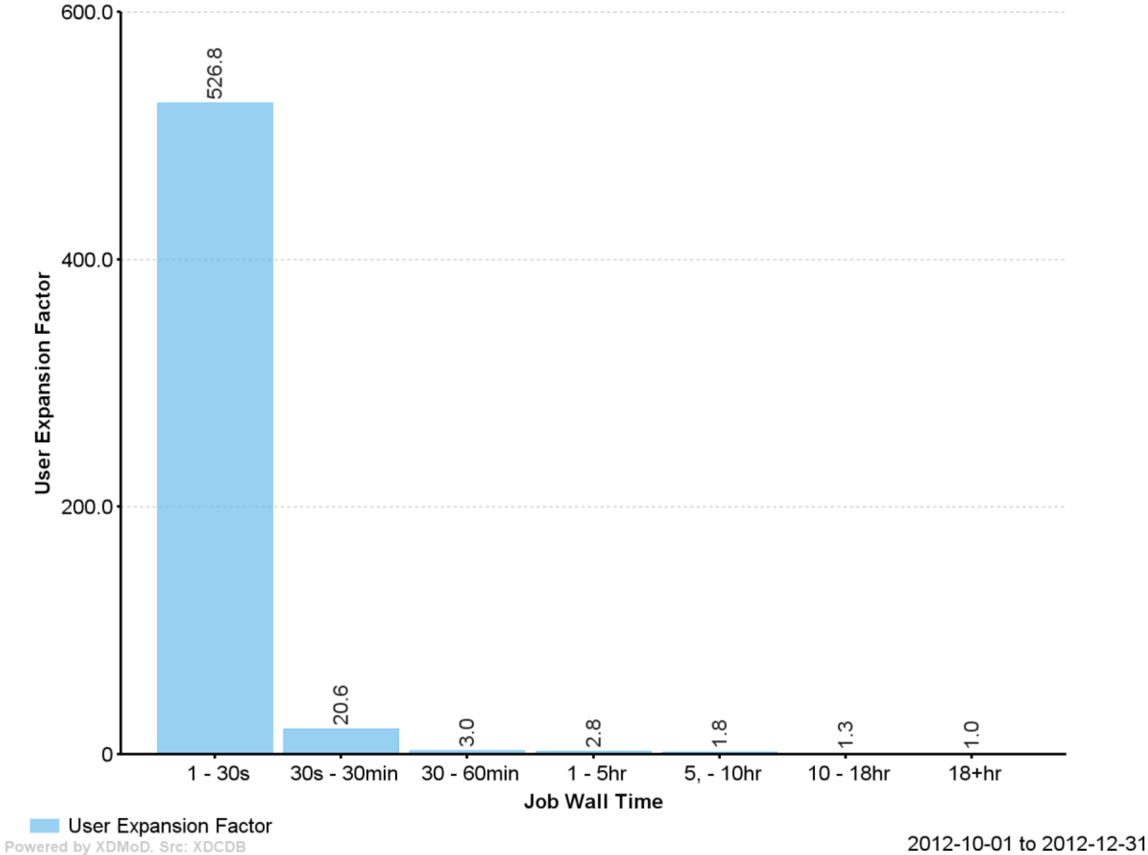
Resource = TACC-LONGHORN

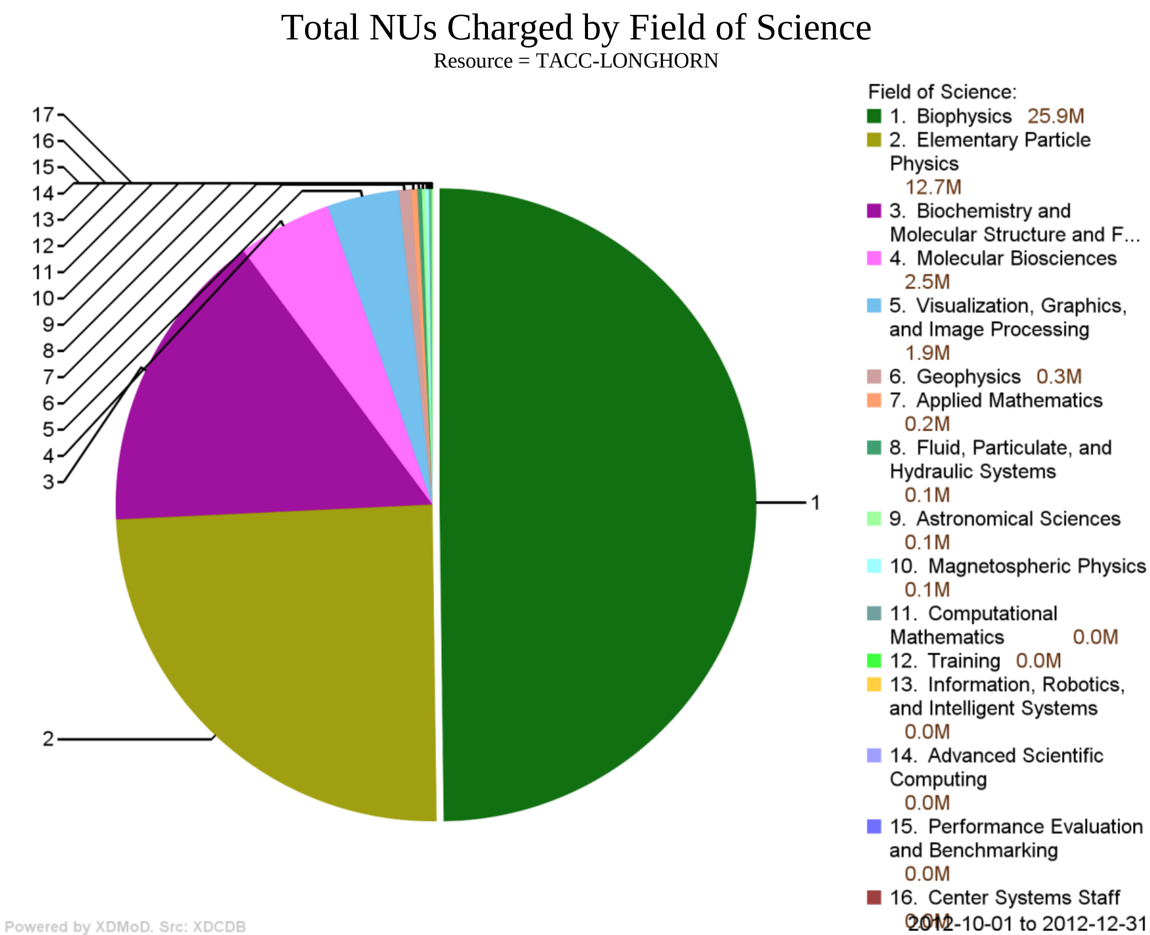



Total NUs Charged by Job Wall Time
Resource = TACC-LONGHORN
30.0M
20.0M
10.0M
0
Total NUs Charged
668.4
259,365.7
501,017.4
5,657,867.8
19,631,698.8
9,512,052.1
16,487,792.1
1 - 30s
30s - 30min
30 - 60min
1 - 5hr
5, - 10hr
10 - 18hr
18+hr
Job Wall Time
Total NUs Charged
Powered by XDMoD. Src: XDCDB
2012-10-01 to 2012-12-31

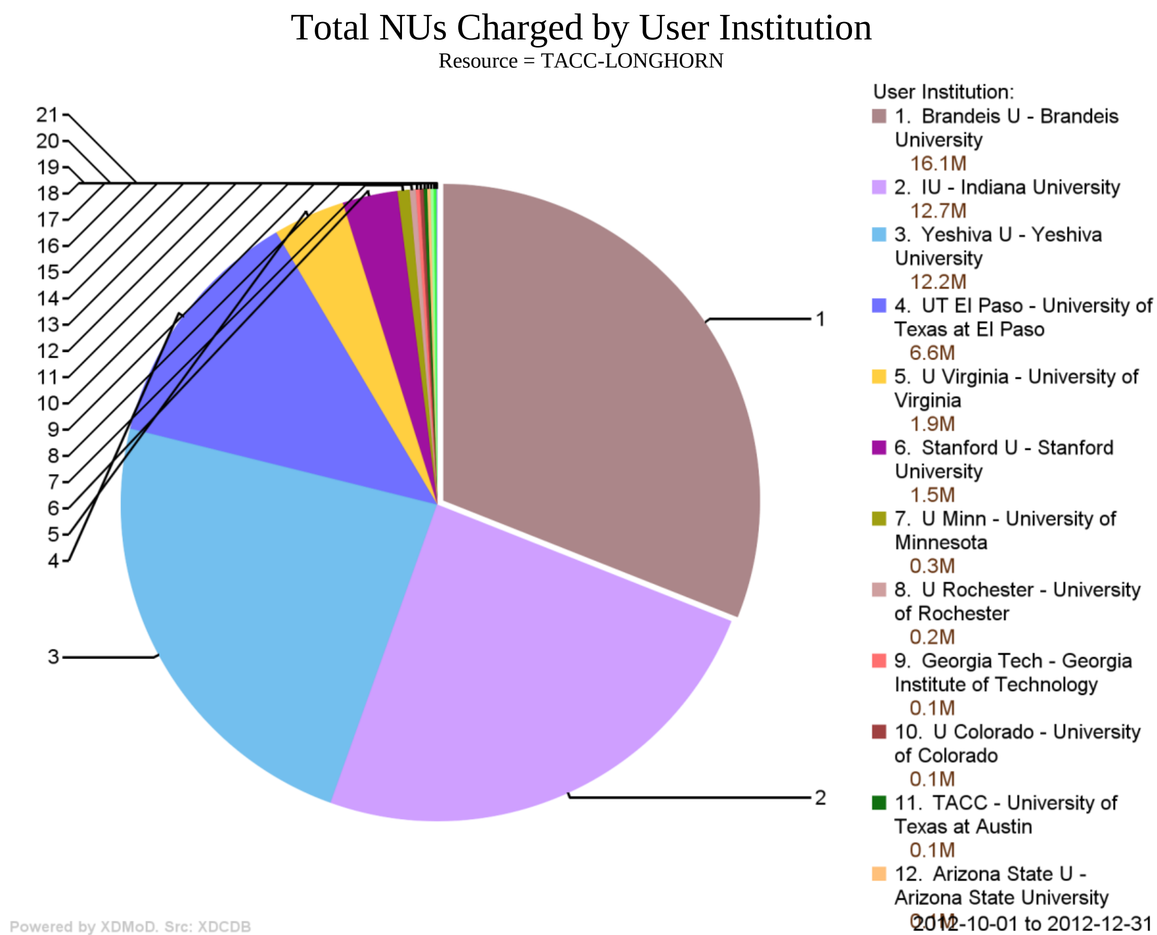
User Expansion Factor by Job Wall Time

Resource = TACC-LONGHORN -- Service Provider = TACC



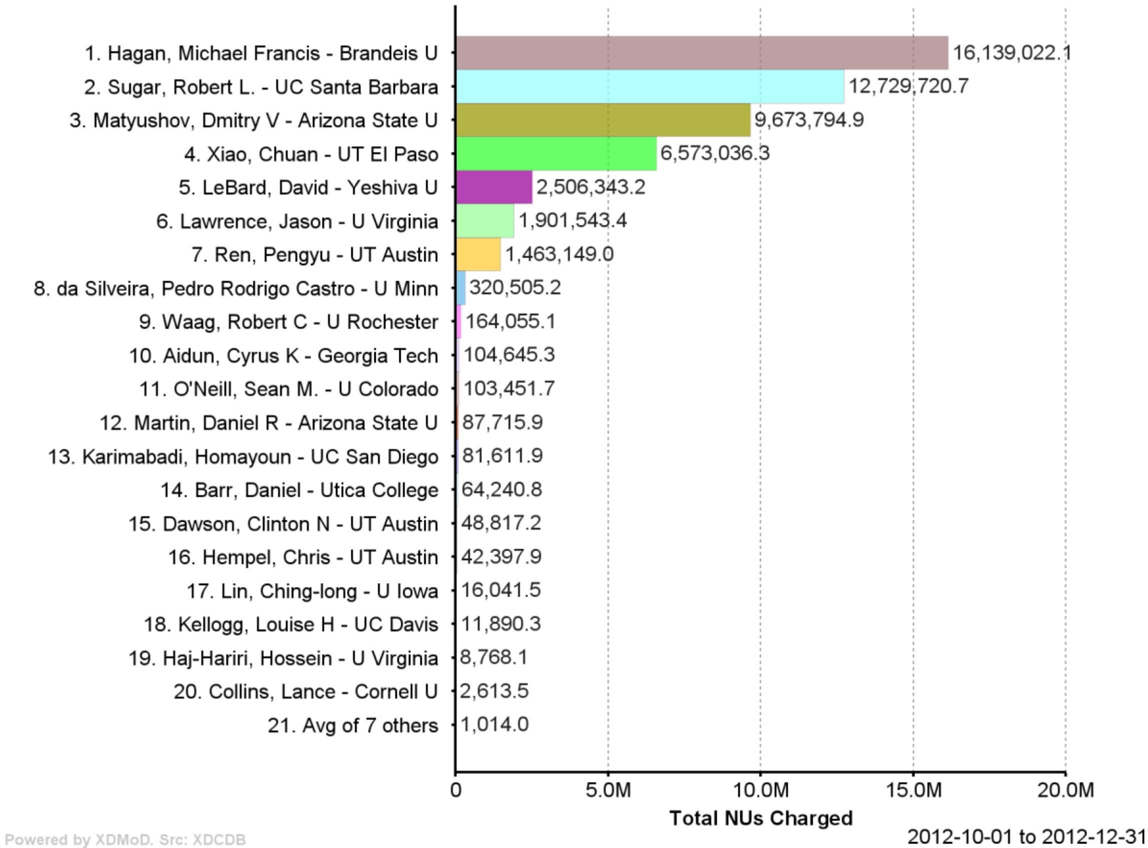


Total NUs Charged by Field of Science
Resource = TACC-LONGHORN
Field of Science:
1. Biophysics 25.9M
2. Elementary Particle Physics 12.7M
3. Biochemistry and Molecular Structure and F...
4. Molecular Biosciences 2.5M
5. Visualization, Graphics, and Image Processing 1.9M
6. Geophysics 0.3M
7. Applied Mathematics 0.2M
8. Fluid, Particulate, and Hydraulic Systems 0.1M
9. Astronomical Sciences 0.1M
10. Magnetospheric Physics 0.1M
11. Computational Mathematics 0.0M
12. Training 0.0M
13. Information, Robotics, and Intelligent Systems 0.0M
14. Advanced Scientific Computing 0.0M
15. Performance Evaluation and Benchmarking 0.0M
16. Center Systems Staff 0.0M
2012-10-01 to 2012-12-31
Powered by XDMoD. Src: XDCDB


Total NUs Charged by User Institution
Resource = TACC-LONGHORN
User Institution:
1. Brandeis U - Brandeis University
16.1M
2. IU - Indiana University
12.7M
3. Yeshiva U - Yeshiva University
12.2M
4. UT El Paso - University of Texas at El Paso
6.6M
5. U Virginia - University of Virginia
1.9M
6. Stanford U - Stanford University
1.5M
7. U Minn - University of Minnesota
0.3M
8. U Rochester - University of Rochester
0.2M
9. Georgia Tech - Georgia Institute of Technology
0.1M
10. U Colorado - University of Colorado
0.1M
11. TACC - University of Texas at Austin
0.1M
12. Arizona State U - Arizona State University
0.1M
2012-10-01 to 2012-12-31
Powered by XDMoD. Src: XDCDB

Total NUs Charged by PI

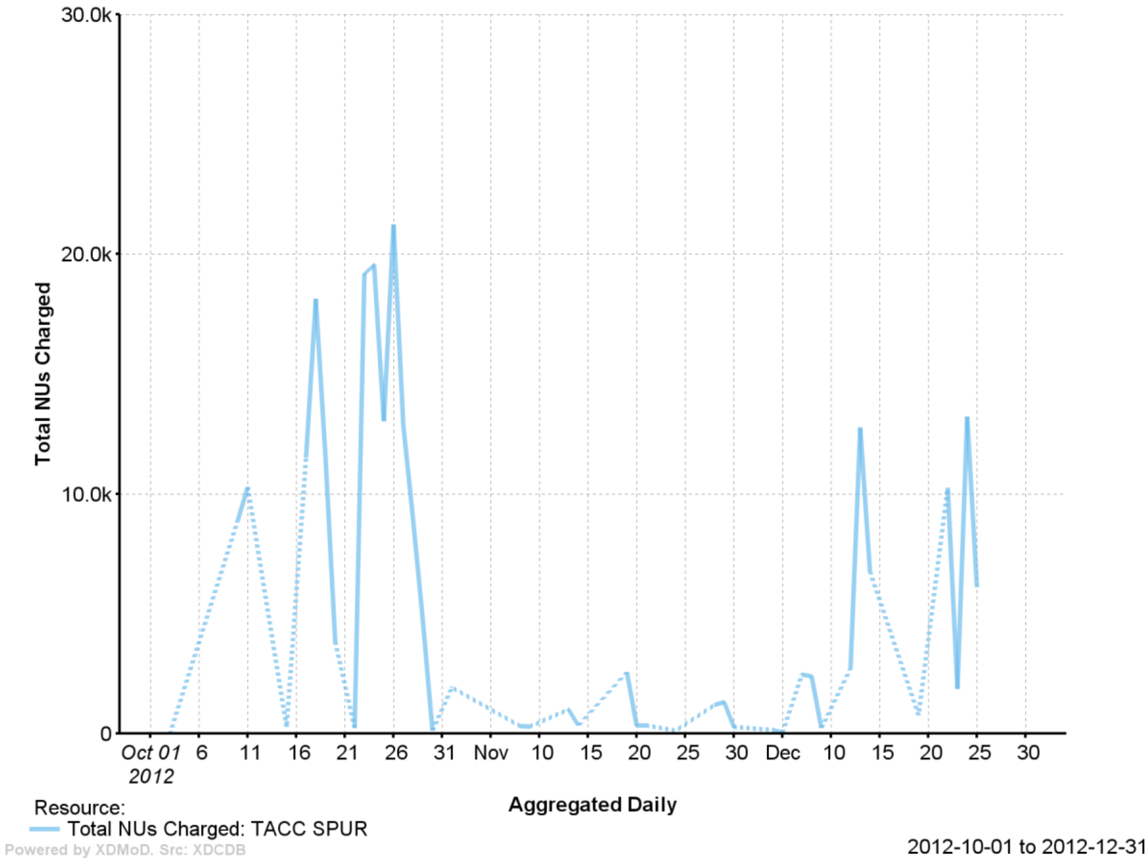
Resource = TACC-LONGHORN

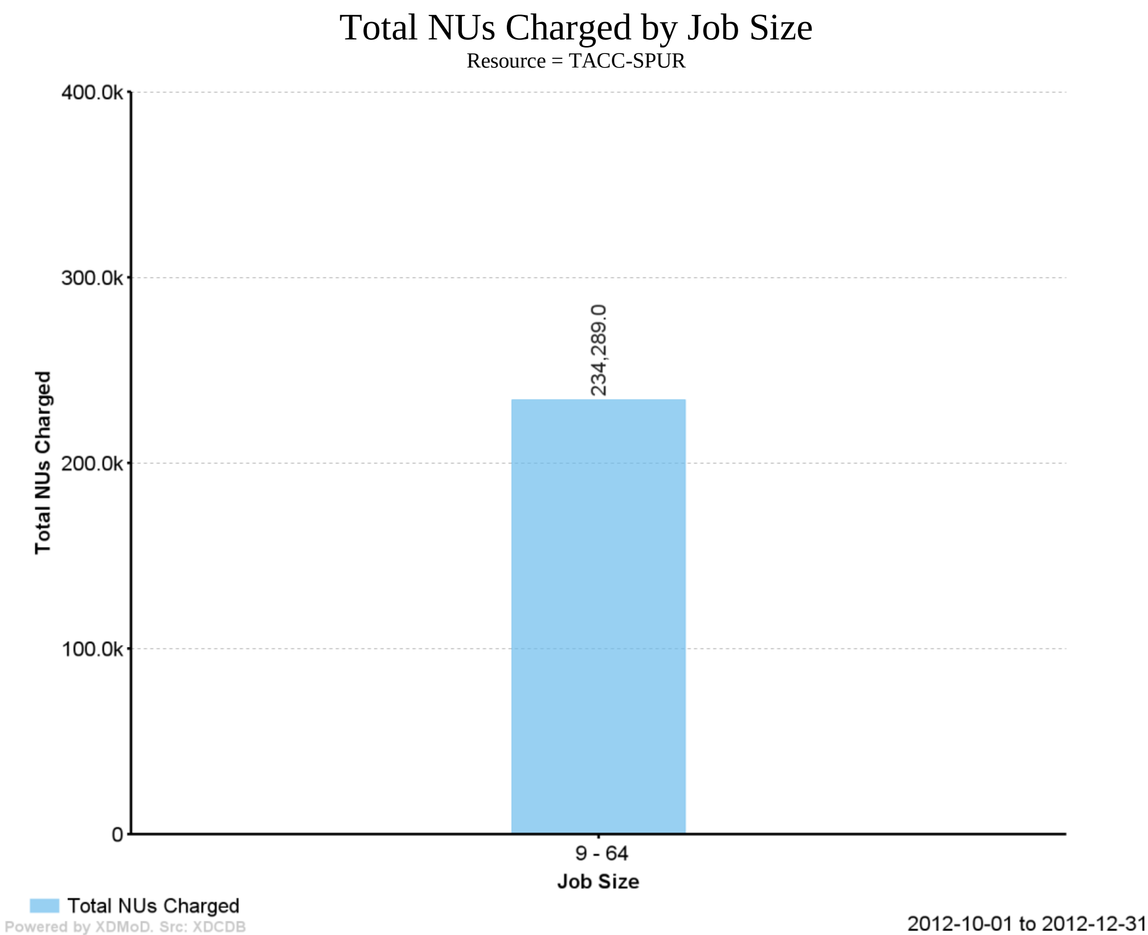


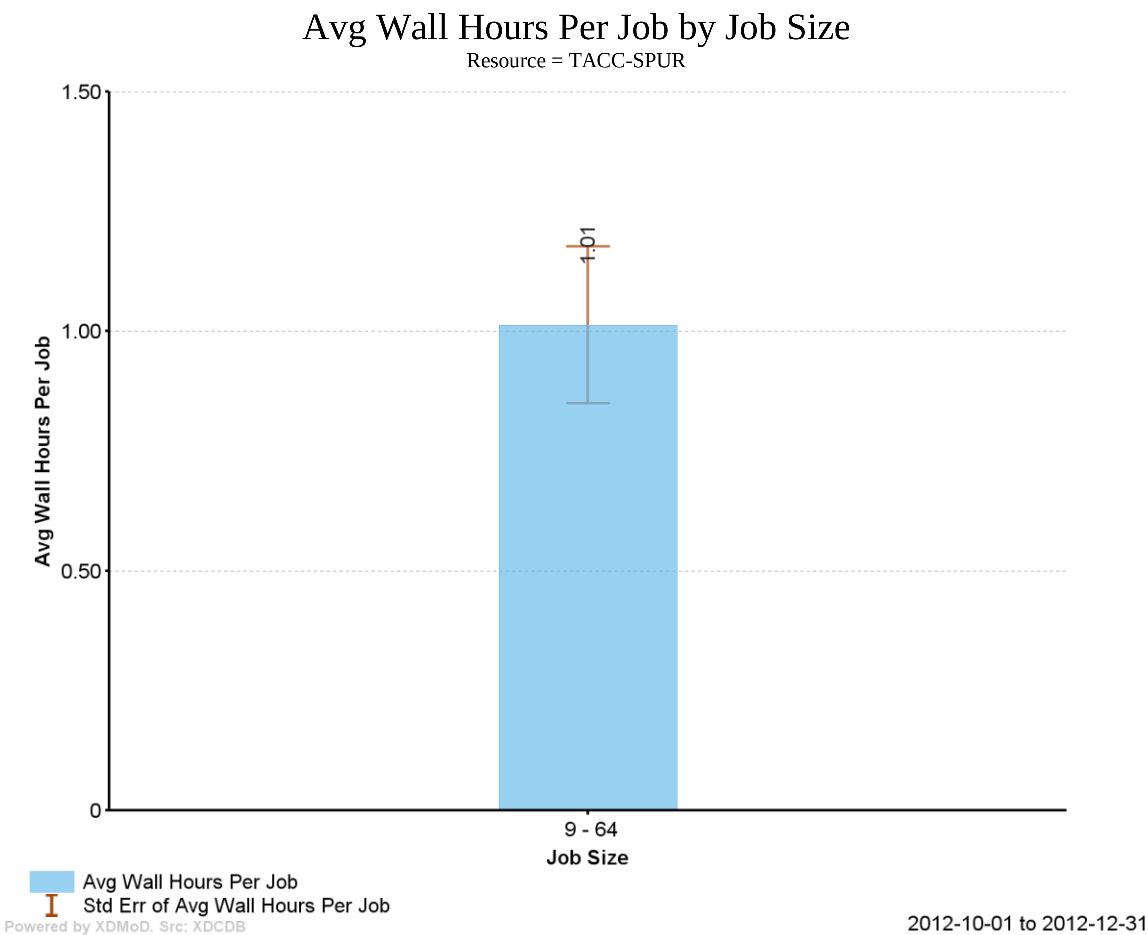
TACC-SPUR Quarterly Report

Total NUs Charged by Resource

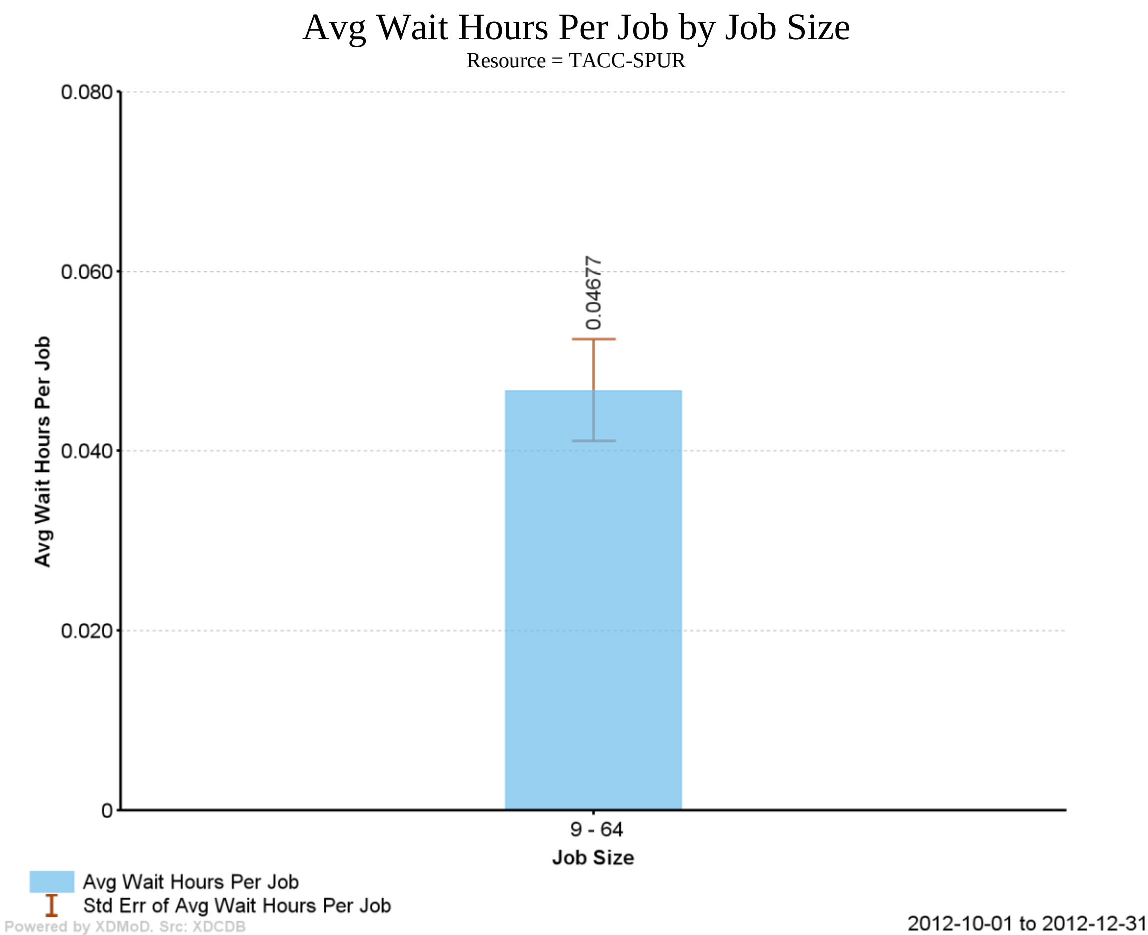
Service Provider = TACC

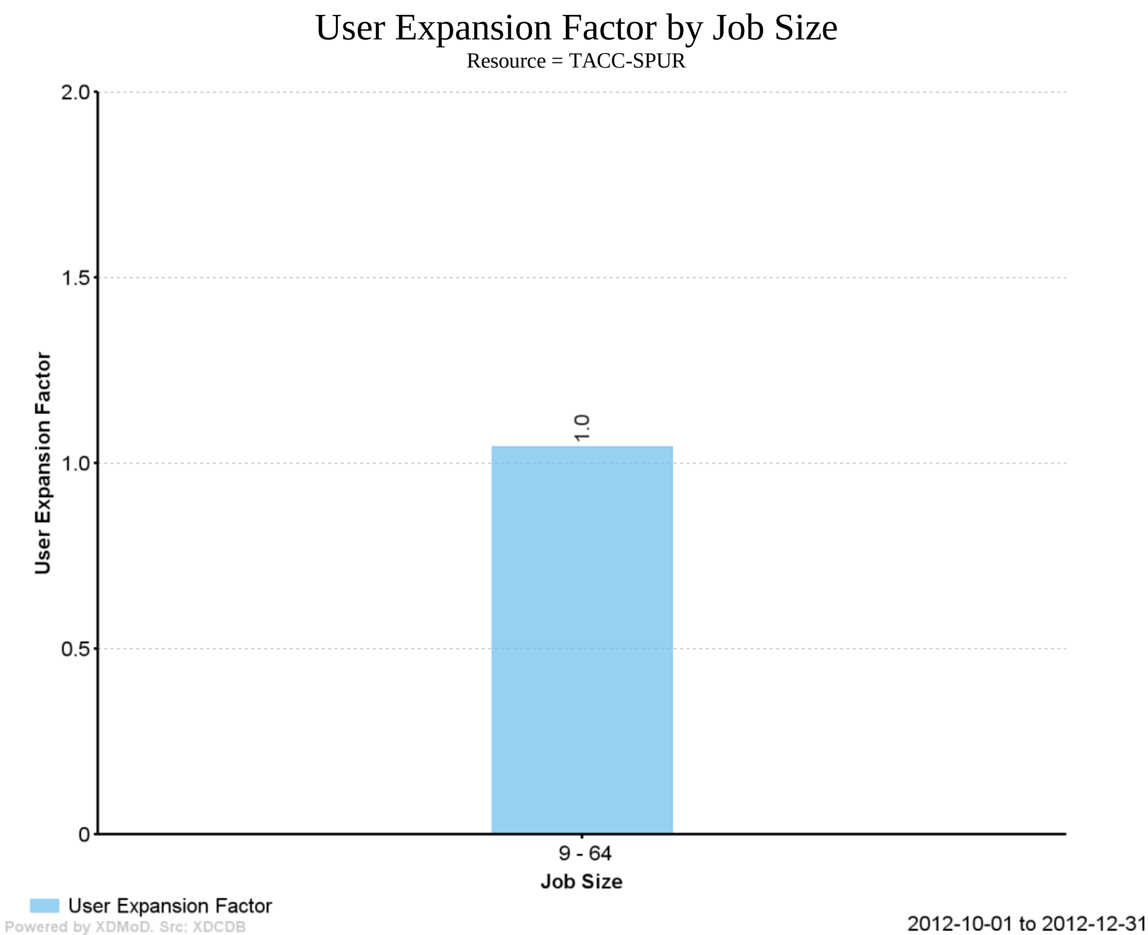


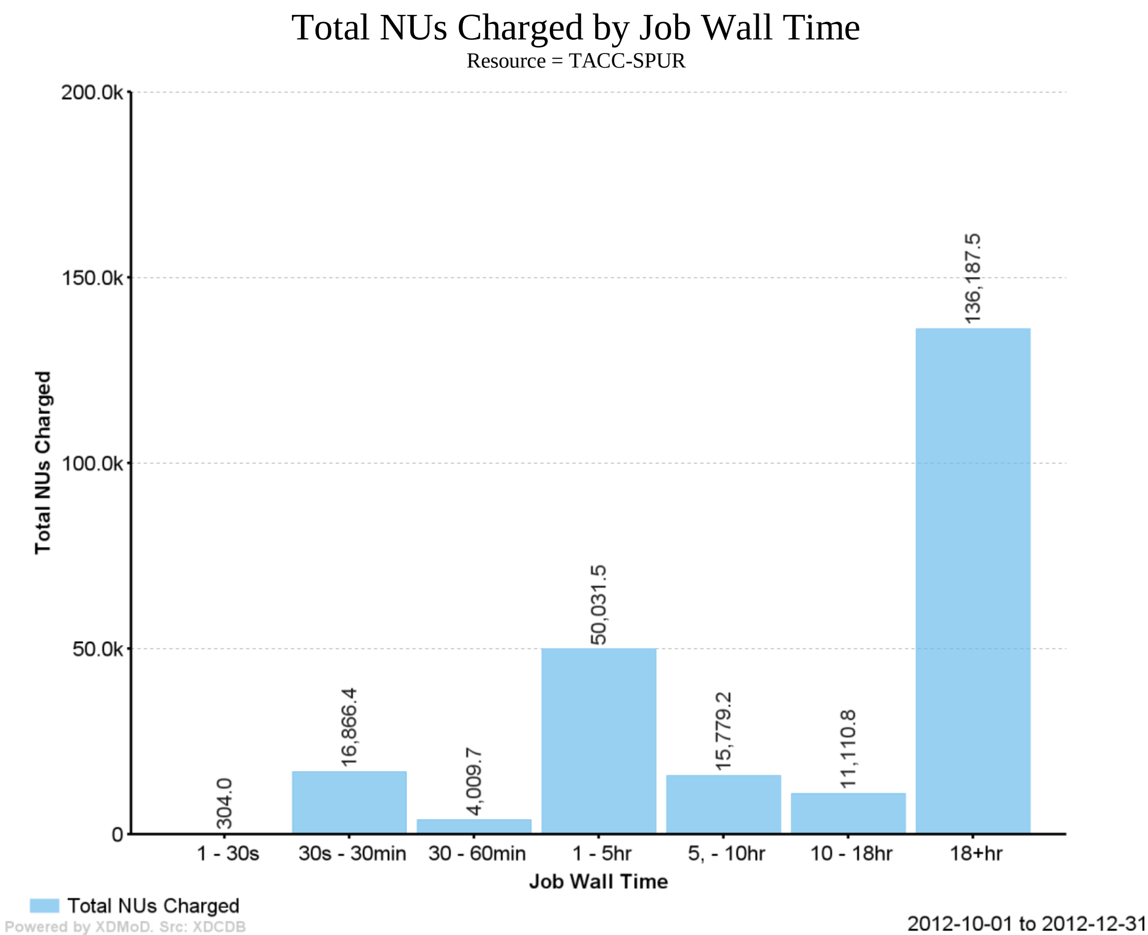

Total NUs Charged by Job Size
Resource = TACC-SPUR
400.0k
300.0k
200.0k
100.0k
0
Total NUs Charged
234,289.0
9 - 64
Job Size
Total NUs Charged
Powered by XDMoD. Src: XDCDB
2012-10-01 to 2012-12-31



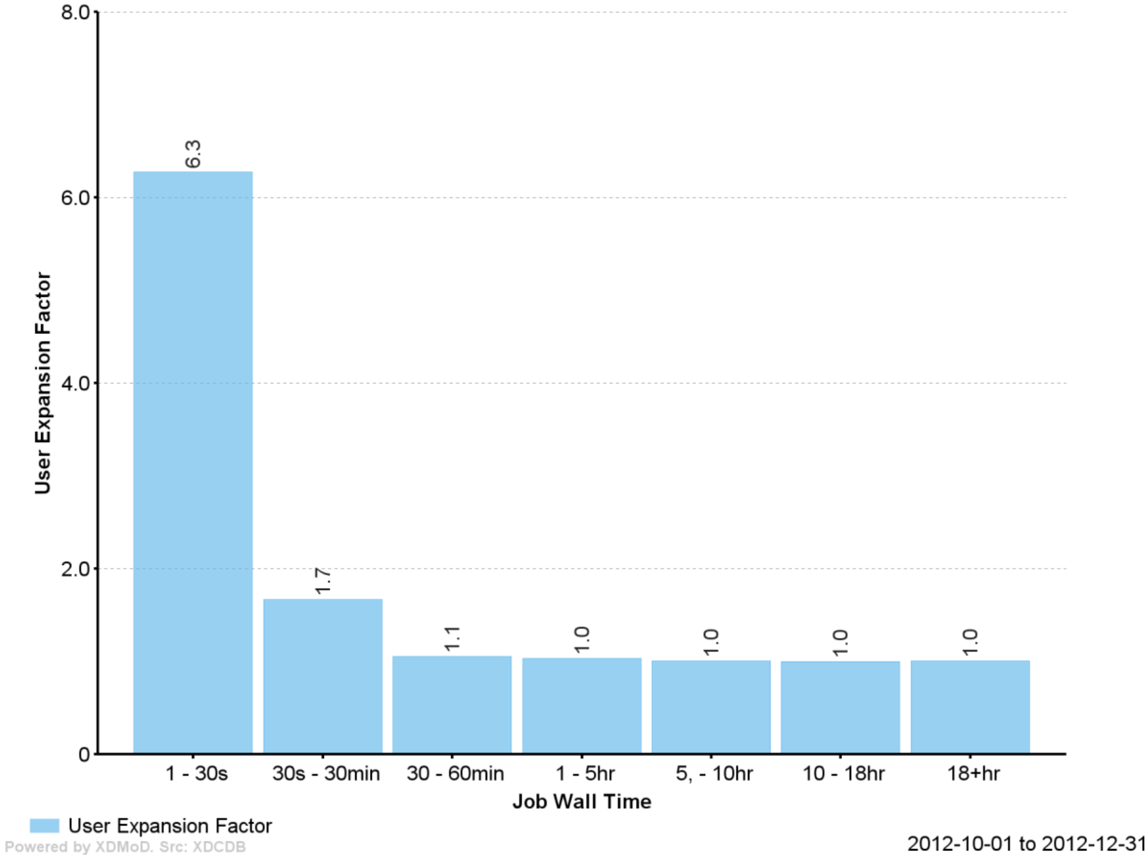
Avg Wall Hours Per Job by Job Size
Resource = TACC-SPUR
1.50
1.00
0.50
0
Avg Wall Hours Per Job
1.01
9 - 64
Job Size
Avg Wall Hours Per Job
Std Err of Avg Wall Hours Per Job
Powered by XDMoD. Src: XDCDB
2012-10-01 to 2012-12-31

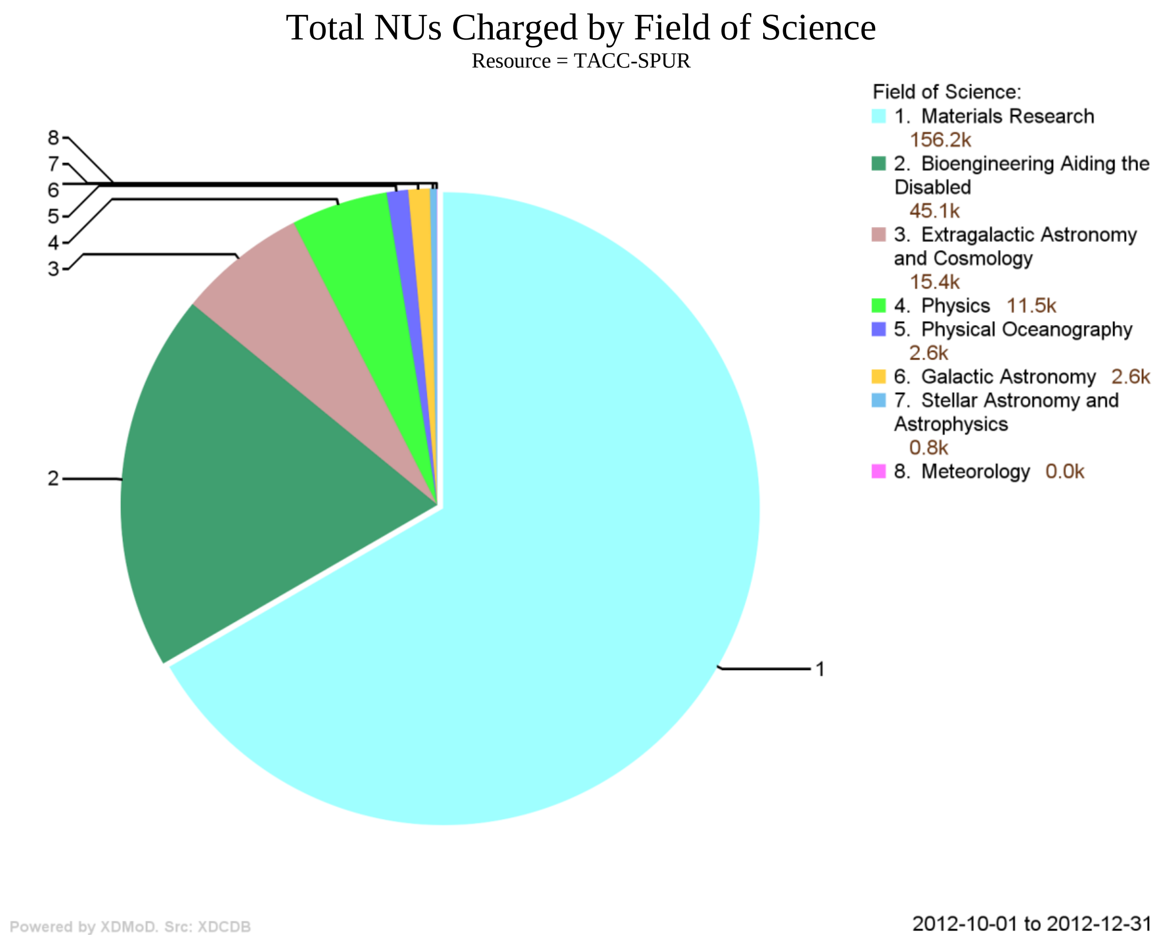

Avg Wait Hours Per Job by Job Size
Resource = TACC-SPUR
0.080
0.060
0.040
0.020
0
Avg Wait Hours Per Job
0.04677
9 - 64
Job Size
Avg Wait Hours Per Job
Std Err of Avg Wait Hours Per Job
Powered by XDMoD. Src: XDCDB
2012-10-01 to 2012-12-31


User Expansion Factor by Job Size
Resource = TACC-SPUR
2.0
1.5
1.0
0.5
0
User Expansion Factor
1.0
9 - 64
Job Size
User Expansion Factor
Powered by XDMoD. Src: XDCDB
2012-10-01 to 2012-12-31


Total NUs Charged by Job Wall Time
Resource = TACC-SPUR
200.0k
150.0k
100.0k
50.0k
0
Total NUs Charged
304.0
16,866.4
4,009.7
50,031.5
15,779.2
11,110.8
136,187.5
1 - 30s
30s - 30min
30 - 60min
1 - 5hr
5, - 10hr
10 - 18hr
18+hr
Job Wall Time
Total NUs Charged
Powered by XDMoD. Src: XDCDB
2012-10-01 to 2012-12-31

User Expansion Factor by Job Wall Time
Resource = TACC-SPUR -- Service Provider = TACC

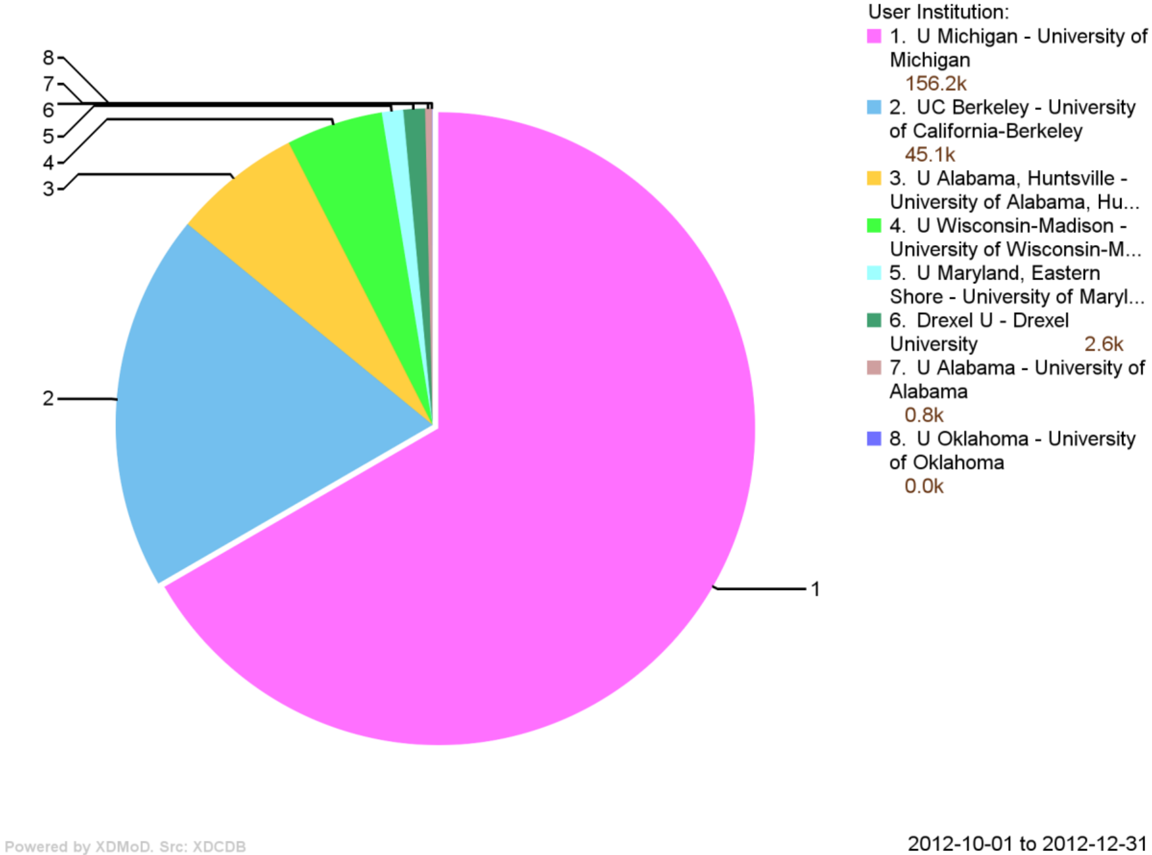




Total NUs Charged by Field of Science
Resource = TACC-SPUR
Field of Science:
1. Materials Research 156.2k
2. Bioengineering Aiding the Disabled 45.1k
3. Extragalactic Astronomy and Cosmology 15.4k
4. Physics 11.5k
5. Physical Oceanography 2.6k
6. Galactic Astronomy 2.6k
7. Stellar Astronomy and Astrophysics 0.8k
8. Meteorology 0.0k
1
2
3
4
5
6
7
8
Powered by XDMoD. Src: XDCDB
2012-10-01 to 2012-12-31

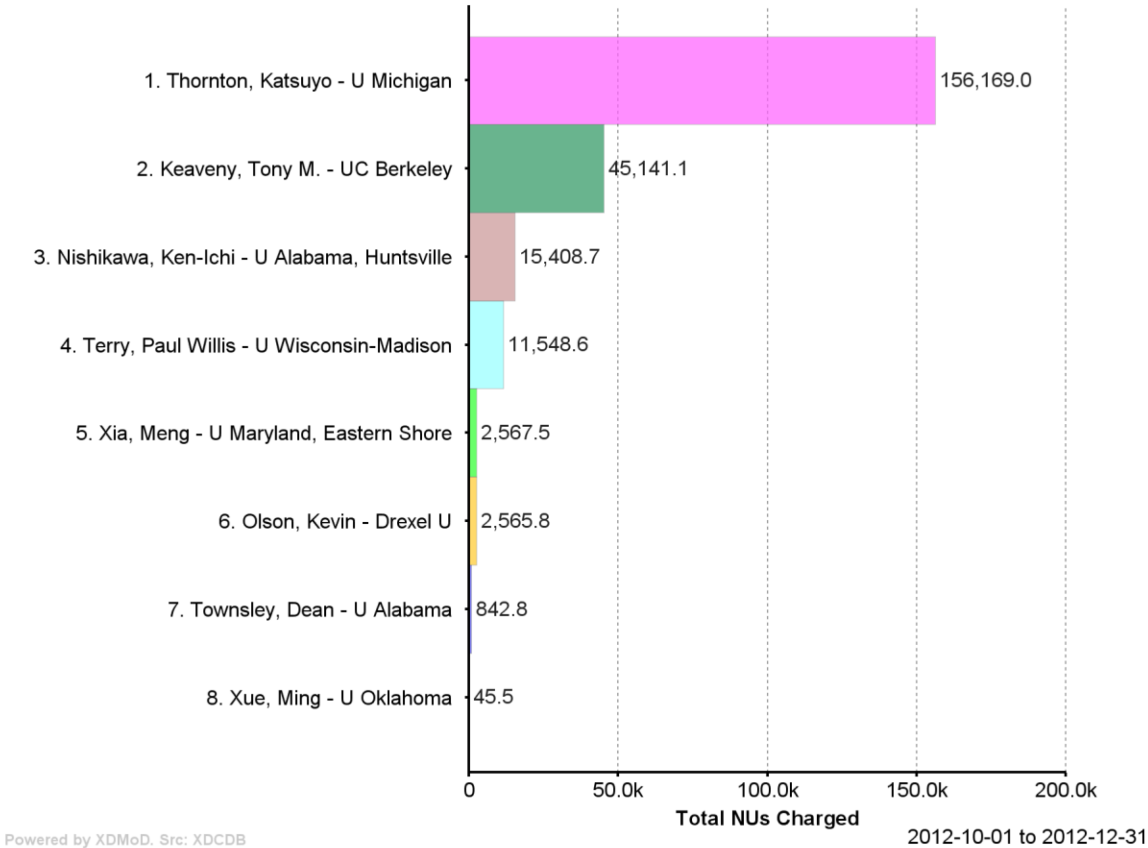
Total NUs Charged by User Institution

Resource = TACC-SPUR



Total NUs Charged by PI

Resource = TACC-SPUR

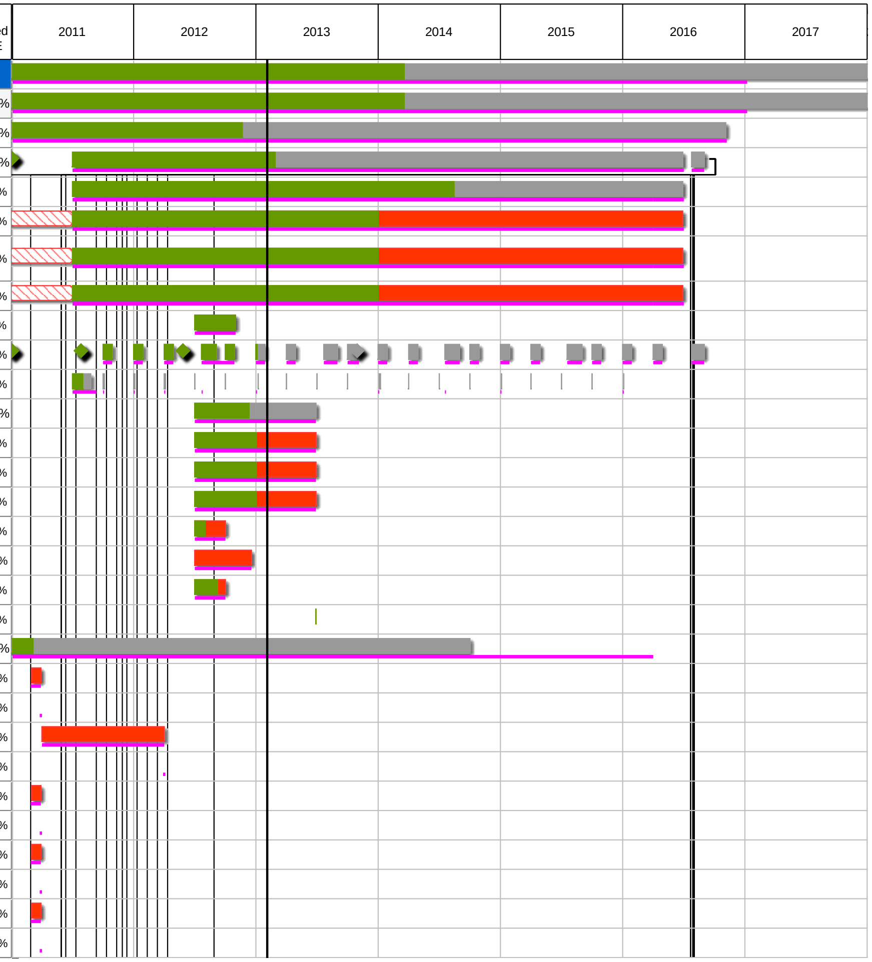


A XSEDE Project Milestones Update

Content for this appendix is pending finalizing the XSEDE Architecture that is being reworked due to the merging of the XSEDE and XROADS proposals.

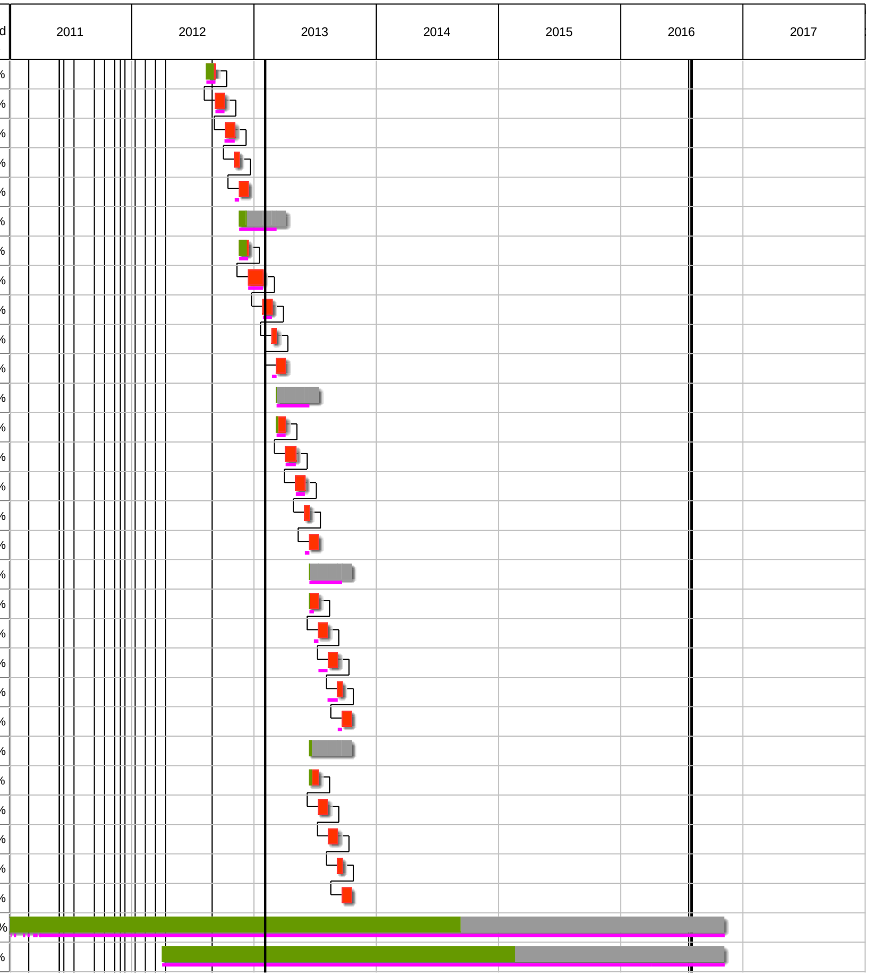
B XSEDE Schedule with Progress Update

Name	Start	Finish	% Completed - XSEDE
Prodution: XSEDE Schedule	**10/6/10**	**7/9/21**	
XSEDE	10/6/10	7/9/21	32.05%
Project Office	10/6/10	11/3/16	34.99%
Project Management and Reporting	10/6/10	8/31/16	33.58%
Management	7/1/11	6/29/16	62.50%
Ongoing: Senior Management Team - Oversight and management of XSEDE	7/1/11	6/29/16	50.00%
Ongoing: Business and finance office support - subaward management	7/1/11	6/29/16	50.00%
Ongoing: Annual Planning, Budgeting, Change Control resulting from SEMP	7/1/11	6/29/16	50.00%
Update Project Execution Plan	7/2/12	10/31/12	100.00%
Project Reporting	10/6/10	8/31/16	28.57%
Project Management - Risk Management	7/1/11	1/5/16	38.10%
Systems Engineering	7/2/12	6/28/13	44.29%
User needs collection	7/2/12	6/28/13	50.00%
Requirements analysis	7/2/12	6/28/13	50.00%
Managing the UREP	7/2/12	6/28/13	50.00%
Updating the Requirements Management Plan	7/2/12	9/28/12	35.00%
Updating the SEMP	7/2/12	12/14/12	0.00%
XDOR/IDEALS: establishing procedures/developing documentation	7/2/12	9/28/12	75.00%
Management of XDOR process	6/28/13	6/28/13	50.00%
Systems Architecture	10/6/10	9/30/14	10.37%
Deploy Grid Middleware Infrastructure	3/1/11	3/28/11	0.00%
Milestone: Grid Middleware Infrastructure deployed	10/6/10	10/6/10	0.00%
Deploy Data Management software	4/1/11	3/29/12	0.00%
Milestone: Data Management software deployed	10/6/10	10/6/10	0.00%
Deploy Account Management software	3/1/11	3/28/11	0.00%
Milestone: Account Management software deployed	10/6/10	10/6/10	0.00%
Deploy Information Services Infrastructure	3/1/11	3/28/11	0.00%
Milestone: Information Services Infrastructure deployed	10/6/10	10/6/10	0.00%
Deploy Common User Environment	3/1/11	3/28/11	0.00%
Milestone: Common User Environment deployed	10/6/10	10/6/10	0.00%



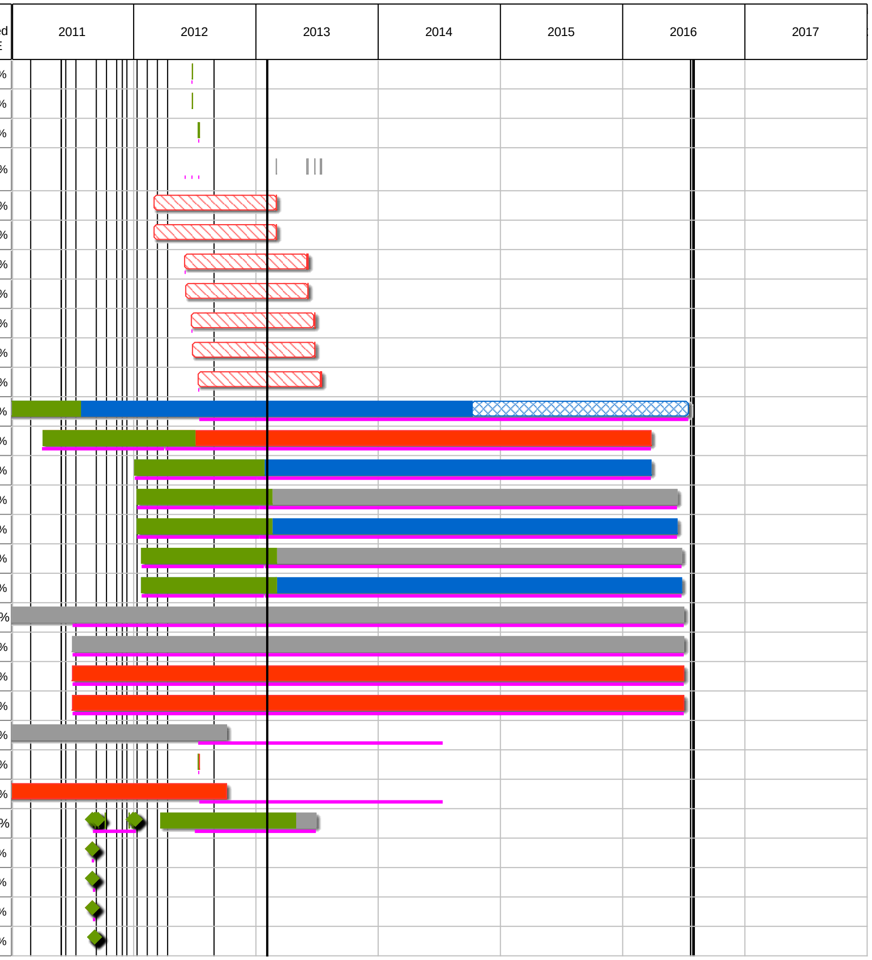
Name	Start	Finish	% Completed - XSEDE
Deploy System of Systems Test Environment	3/1/11	3/28/11	0.00%
Milestone: System of Systems Test Environment deployed	10/6/10	10/6/10	0.00%
Spiral 1.0	1/3/11	12/21/11	0.00%
Spiral 2.0	5/3/11	10/18/11	0.00%
Spiral 3.0	10/18/11	4/4/12	0.00%
Ongoing: Incremental improvements continue via SEMP Spiral Design Process	10/6/10	9/30/14	0.00%
Public Facing XSEDE Architecture Document	12/5/11	3/5/12	100.00%
Agreement of contents and level of detail	12/5/11	12/8/11	100.00%
Establish time frame to produce public facing architecture document	12/9/11	1/5/12	100.00%
Outline for initial level 1 & level 2-decomposition documentation	1/6/12	1/12/12	100.00%
First draft of public facing document	1/13/12	2/1/12	100.00%
Revise, comment add content to document as necessary	2/2/12	2/9/12	100.00%
Architects review first draft with Bachman	2/10/12	2/10/12	100.00%
Identify remaining steps to complete first draft	2/13/12	2/16/12	100.00%
A&D team including liaisons from SD&I, Security, Campus Bridging and	2/17/12	2/27/12	100.00%
Architects address comments/revisions and request endorsement from A&D	2/28/12	3/1/12	100.00%
First version of XSEDE Architecture Document (Level 1 & 2 Decomp)	3/2/12	3/5/12	100.00%
Campus Bridging - Architectural Response to Stakeholder Requirements	1/19/12	5/31/12	65.00%
Preliminary background work	1/19/12	2/16/12	100.00%
Documentation and review of use cases and requirements matrix completed	2/17/12	2/23/12	100.00%
Architectural response at a Level 3 Decomposition prepared by the	2/24/12	3/22/12	95.00%
Stakeholder review of Architectural response	3/23/12	4/19/12	95.00%
Active Design Review	4/20/12	5/3/12	0.00%
Incorporation into public facing XSEDE Architecture Document	5/4/12	5/31/12	0.00%
Science Gateways - Architectural Response to Stakeholder Requirements	5/4/12	9/6/12	18.00%
Documentation and review of use cases and requirements matrix completed	5/4/12	5/31/12	90.00%
Architectural response at a Level 3 Decomposition prepared by the	6/1/12	6/28/12	0.00%
Stakeholder review of Architectural response	6/29/12	7/26/12	0.00%
Active Design Review	7/27/12	8/9/12	0.00%
Incorporation into public facing XSEDE Architecture Document	8/10/12	9/6/12	0.00%
Computing - Architectural Response to Stakeholder Requirements	8/10/12	12/13/12	16.00%

Name	Start	Finish	% Completed - XSEDE
Documentation and review of use cases and requirements matrix completed	8/10/12	9/6/12	80.00%
Architectural response at a Level 3 Decomposition prepared by the	9/7/12	10/4/12	0.00%
Stakeholder review of Architectural response	10/5/12	11/1/12	0.00%
Active Design Review	11/2/12	11/15/12	0.00%
Incorporation into public facing XSEDE Architecture Document	11/16/12	12/13/12	0.00%
⊟ BIG Data - Architectural Response to Stakeholder Requirements	11/16/12	4/4/13	15.00%
Documentation and review of use cases and requirements matrix completed	11/16/12	12/13/12	75.00%
Architectural response at a Level 3 Decomposition prepared by the	12/14/12	1/25/13	0.00%
Stakeholder review of Architectural response	1/28/13	2/21/13	0.00%
Active Design Review	2/22/13	3/7/13	0.00%
Incorporation into public facing XSEDE Architecture Document	3/8/13	4/4/13	0.00%
⊟ Connecting Instrumentation - Architectural Response to Stakeholder Requirements	3/8/13	7/11/13	1.00%
Documentation and review of use cases and requirements matrix completed	3/8/13	4/4/13	5.00%
Architectural response at a Level 3 Decomposition prepared by the	4/5/13	5/2/13	0.00%
Stakeholder review of Architectural response	5/3/13	5/30/13	0.00%
Active Design Review	5/31/13	6/13/13	0.00%
Incorporation into public facing XSEDE Architecture Document	6/14/13	7/11/13	0.00%
⊟ Collaboration - Architectural Response to Stakeholder Requirements	6/14/13	10/17/13	1.00%
Documentation and review of use cases and requirements matrix completed	6/14/13	7/11/13	5.00%
Architectural response at a Level 3 Decomposition prepared by the	7/12/13	8/8/13	0.00%
Stakeholder review of Architectural response	8/9/13	9/5/13	0.00%
Active Design Review	9/6/13	9/19/13	0.00%
Incorporation into public facing XSEDE Architecture Document	9/20/13	10/17/13	0.00%
⊟ XSEDE Architectural Canonical Use Cases	6/14/13	10/17/13	5.00%
Documentation and review of use cases and requirements matrix completed	6/14/13	7/11/13	25.00%
Architectural response at a Level 3 Decomposition prepared by the	7/12/13	8/8/13	0.00%
Stakeholder review of Architectural response	8/9/13	9/5/13	0.00%
Active Design Review	9/6/13	9/19/13	0.00%
Incorporation into public facing XSEDE Architecture Document	9/20/13	10/17/13	0.00%
⊟ External Relations	10/6/10	11/3/16	64.52%
⊟ Generate Publications: Highlights (Science, EOT, Digital Resources)	4/2/12	11/3/16	62.73%



Name	Start	Finish	% Completed - XSEDE
SciHi subcommittee from XSEDE ER established	4/9/12	4/9/12	100.00%
Collect story ideas	5/25/12	5/25/12	100.00%
Story choices approved by XSEDE leadership	6/29/12	6/29/12	100.00%
Graphic designer selected	7/2/12	7/2/12	100.00%
About 15 science highlights stories selected, edited (incl tech review) and	7/27/12	7/27/12	100.00%
Cover-to-cover edit complete	8/10/12	8/10/12	100.00%
Overall design and test story mockup complete and reviewed	9/5/12	9/5/12	90.00%
Final design complete	9/20/12	9/20/12	0.00%
Completed book delivered to printer	9/21/12	9/21/12	0.00%
Milestone: Science Highlights published	11/21/12	11/21/12	0.00%
Ongoing: Repeat previous 10 tasks annually	4/2/12	11/3/16	0.00%
Create XSEDE website and translate relevant TG website content	1/3/11	4/18/11	100.00%
XSEDE WebsiXSEDE website committee established	1/3/11	1/3/11	100.00%
Website requirements document complete	1/17/11	1/17/11	100.00%
Content requirements document complete	1/17/11	1/17/11	100.00%
First rev of design reviewed by website committee	2/15/11	2/15/11	100.00%
Rev of website reviewed by XSEDE leadership	3/1/11	3/1/11	100.00%
Short form usability test completed	3/15/11	3/15/11	100.00%
Final version of website reviewed by website committee	3/22/11	3/22/11	100.00%
Content approved	4/1/11	4/1/11	100.00%
Final build complete	4/7/11	4/7/11	100.00%
Content ported and built	4/15/11	4/15/11	100.00%
Initial version of XSEDE website launched	4/18/11	4/18/11	100.00%
Milestone: XSEDE website completed	4/18/11	4/18/11	100.00%
Generate Annual Conference Proceedings	10/6/10	10/7/14	48.00%
Genereate Annual Conference 2012	3/1/12	7/12/12	100.00%
Proceedings chair selected and incorporated into event planning	3/1/12	3/1/12	100.00%
Submission site publicized	3/1/12	3/1/12	100.00%
Approval from ACM or whatever publisher received	6/1/12	6/1/12	100.00%
Templates and copyright permission forms out to authors	6/5/12	6/5/12	100.00%

Name	Start	Finish	% Completed - XSEDE
All papers and copyright permission forms received from authors and	6/22/12	6/22/12	100.00%
All papers sent to production house for reproduction to USB drive	6/25/12	6/25/12	100.00%
Milestone: Annual Conference Proceedings Complete	7/12/12	7/12/12	100.00%
Genereate Annual Conference 2013	3/1/13	7/12/13	0.00%
Proceedings chair selected and incorporated into event planning	3/1/13	3/1/13	0.00%
Submission site publicized	3/1/13	3/1/13	0.00%
Approval from ACM or whatever publisher received	6/1/13	6/3/13	0.00%
Templates and copyright permission forms out to authors	6/5/13	6/5/13	0.00%
All papers and copyright permission forms received from authors and	6/22/13	6/24/13	0.00%
All papers sent to production house for reproduction to USB drive	6/25/13	6/25/13	0.00%
Milestone: Annual Conference Proceedings Complete	7/12/13	7/12/13	0.00%
Ongoing: Repeat previous 7 tasks annually	10/6/10	10/7/14	20.00%
Milestone: Ongoing - Generate press releases & website content	4/4/11	3/24/16	25.00%
Milestone: Ongoing - Generate publicity via social media	1/3/12	3/24/16	25.00%
Monthly: Gather, edit and format content for internal (plain text) e-newsletter; distribute to	1/10/12	6/9/16	25.00%
Milestone: Ongoing - Generate monthly internal e-newsletter	1/10/12	6/9/16	25.00%
Monthly: Gather, edit and format content for external (HTML/designed) e-newsletter;	1/25/12	6/23/16	25.00%
Milestone: Ongoing - Generate monthly external e-newsletter	1/25/12	6/23/16	25.00%
Industry Relations	10/6/10	6/30/16	0.25%
Workforce Development	7/1/11	6/30/16	0.00%
Increase industry partners' awareness of all XSEDE SP's training opportunites	7/1/11	6/30/16	0.00%
Elicit industry partners' input to enhance training programs for workforce	7/1/11	6/30/16	0.00%
Software Development	10/6/10	10/2/12	0.50%
Hold conference call with XAB to flesh out software development activity	7/12/12	7/12/12	1.00%
Select and execute the software development project	10/6/10	10/2/12	0.00%
SD&I	9/1/11	6/28/13	86.64%
PDR	9/1/11	9/1/11	100.00%
Increment Planning	9/1/11	9/1/11	100.00%
develop incrment plan	9/1/11	9/1/11	100.00%
IRR	9/7/11	9/7/11	100.00%



Name	Start	Finish	% Completed - XSEDE	2011	2012	2013	2014	2015	2016	2017
conduct IRR	9/7/11	9/7/11	100.00%							
IRR complete and passed	9/7/11	9/7/11	100.00%							
CI Detailed Design	9/8/11	9/8/11	100.00%							
develop detail design	9/8/11	9/8/11	100.00%							
GFFS	9/8/11	9/8/11	100.00%							
Execution Management	9/8/11	9/8/11	100.00%							
XUAS Data	9/8/11	9/8/11	100.00%							
CDR	9/9/11	9/15/11	100.00%							
conduct CDR	9/9/11	9/9/11	100.00%							
CDR complete and passed	9/15/11	9/15/11	100.00%							
CI Development	9/16/11	9/16/11	100.00%							
develop CI	9/16/11	9/16/11	100.00%							
GFFS	9/16/11	9/16/11	100.00%							
Execution Management	9/16/11	9/16/11	100.00%							
XUAS Data	9/16/11	9/16/11	100.00%							
CI TRR	9/19/11	10/7/11	100.00%							
conduct CI TRR	9/19/11	9/19/11	100.00%							
GFFS	9/19/11	9/19/11	100.00%							
Execution Management	9/19/11	9/19/11	100.00%							
XUAS Data	9/19/11	9/19/11	100.00%							
CI TRR complete and passed	10/7/11	10/7/11	100.00%							
CI Tests	10/10/11	12/15/11	100.00%							
conduct Ci tests	10/10/11	10/10/11	100.00%							
GFFS	10/10/11	10/10/11	100.00%							
Execution Management	10/10/11	10/10/11	100.00%							
XUAS Data	10/10/11	10/10/11	100.00%							
CI Tests complete and passed	12/15/11	12/15/11	100.00%							
STRR	12/16/11	12/16/11	100.00%							
conduct STRR	12/16/11	12/16/11	100.00%							
STRR complete and passed	12/16/11	12/16/11	100.00%							
System Integration Test	12/19/11	12/28/11	100.00%							

Name	Start	Finish	% Completed - XSEDE	2011	2012	2013	2014	2015	2016	2017
conduct system test	12/19/11	12/19/11	100.00%							
System test complete and passed	12/28/11	12/28/11	100.00%							
ORR	12/29/11	12/29/11	100.00%							
conduct ORR	12/29/11	12/29/11	100.00%							
ORR complete and passed	12/29/11	12/29/11	100.00%							
Increment De-brief	12/30/11	1/6/12	100.00%							
increment reflection workshop	12/30/11	12/30/11	100.00%							
reflection and practice report	1/2/12	1/2/12	100.00%							
de-brief complete	1/6/12	1/6/12	100.00%							
Implement Open, Continuous Planning	7/2/12	6/28/13	100.00%							
Implement Continuous Development and Integration	7/2/12	6/28/13	100.00%							
Implement Engineering Improvements	7/2/12	6/28/13	100.00%							
SDIACT-010 - Deliver Operational Tests with Cis	4/19/12	6/29/12	50.00%							
SDIACT-015 - Genesis II/UNICORE 6 GAML SAML	4/3/12	7/2/12	100.00%							
SDIACT-018 - Replicated/Synchronized stateful resource	4/18/12	6/18/12	100.00%							
SDIACT-028 - (CANCELED): GO Transfer REST API as XSEDE Production service	4/25/12	7/2/12	100.00%							
SDIACT-031 - Improve GridFTP for SPs	4/25/12	7/2/12	100.00%							
SDIACT-043 - Genesis II Documentation	4/30/12	7/2/12	100.00%							
SDIACT-044 - (CANCELED, MERGED with SDIACT-100): Campus bridging beta support	4/30/12	7/2/12	100.00%							
SDIACT-049 - Link Globus Online into XSEDE User Portal	4/25/12	7/2/12	100.00%							
SDIACT-050 - MyProxy OAuth Limited Proxy Support	4/20/12	7/2/12	100.00%							
SDIACT-054 - Register new increment 1 components	4/19/12	6/5/12	50.00%							
SDIACT-073 - System information publishing pilot	4/24/12	6/29/12	20.00%							
SDIACT-075 - GridFTP in UNICORE 6	5/1/12	7/2/12	100.00%							
SDIACT-096 - Identify XSEDE not TeraGrid in resource names for new OSG resource	3/22/12	5/9/12	100.00%							
SDIACT-097 - Basic Execution Service	5/2/12	6/25/12	100.00%							
SDIACT-100 - Globus Online Increment 2 addressing security concerns	4/25/12	7/2/12	100.00%							
SDIACT-101 - EMS and GFFS Increment 2 updates	5/8/12	7/2/12	97.00%							
SCIDACT-071 - Improve cmd line single sign-on access	3/27/12	6/29/12	100.00%							
SDIACT-070 - SSO Hub (CLI)	11/9/12	2/28/13	10.00%							
SDIACT-102 - Replace tgusage w/ xdusage	10/4/12	12/14/12	25.00%							

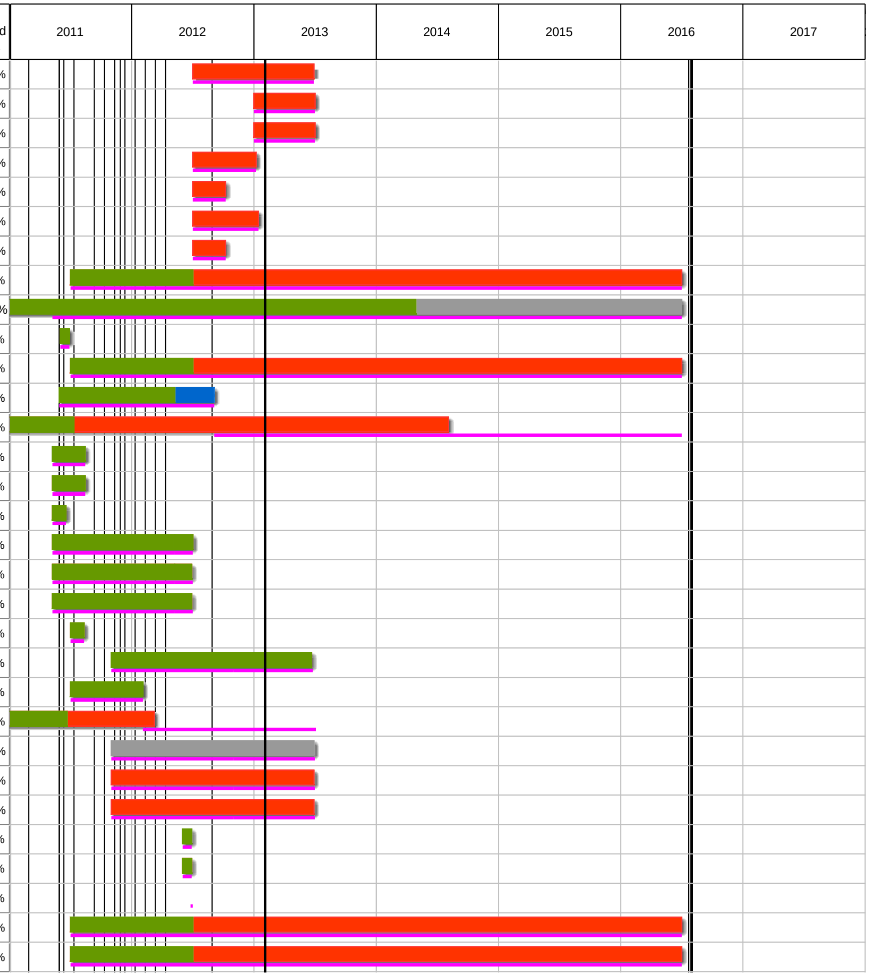
Name	Start	Finish	% Completed - XSEDE
SDIACT-103 - Prototype Acct Mgmt w/ JIRA	11/26/12	1/14/13	50.00%
SDIACT-121 - Activity workspace & process imp.	11/21/12	2/20/13	20.00%
SDIACT-106 Globus Transfer REST APIv1.0	12/5/12	2/14/13	10.00%
SDIACT-108 Globus Connect Multi-user 1.0	12/5/12	2/15/13	10.00%
SDIACT-003 CA Certificate Installer	12/11/12	2/28/13	10.00%
Operations	10/6/10	7/1/16	46.50%
Cybersecurity	10/6/10	7/1/16	40.73%
Setup coordination of XSEDE incident response	5/12/11	7/1/11	100.00%
Setup and deploy XSEDE Certificate Authority	7/1/11	1/4/13	46.00%
Ongoing: Maintain Certificate Authority	10/6/10	10/7/14	20.00%
Develop and deploy Security Awareness program	7/1/11	6/27/13	100.00%
Ongoing: Maintain Security Awareness program	7/2/12	7/1/16	20.00%
Develop and deploy two factor authentication service	10/6/10	5/4/12	50.00%
Evaluate Implementation Options	7/1/11	5/4/12	100.00%
Deploy two factor authentication	10/6/10	6/14/11	0.00%
Ongoing: Maintain two factor authentication service	1/21/13	7/1/16	0.00%
Integrate and deploy InCommon Federated Authentication service	7/1/11	8/23/12	20.00%
Ongoing: Maintain InCommon Federated Authentication service	10/6/10	8/12/14	0.00%
Ongoing: Develop and implement improvements based on SEMP Spiral Design	7/1/11	6/30/16	20.00%
Ongoing: XSEDE Incident response	7/1/11	6/30/16	20.00%
Ongoing: Conduct on-demand security reviews for SD&I	7/2/12	6/30/16	15.00%
Ongoing: Conduct security reviews for ST&D	7/2/12	7/1/16	15.00%
Conduct XSEDE security risk assessment	7/2/12	12/21/12	100.00%
Setup XSEDE Nessus vulnerability assessment capability	9/3/12	12/14/12	100.00%
Setup secure wiki	7/2/12	8/24/12	100.00%
Install and update intrusion detection capability and security monitoring	9/3/12	2/15/13	0.00%
Obtain InCommon membership for XSEDE	3/1/12	8/14/12	100.00%
Conduct annual XSEDE security meeting	6/28/13	7/2/13	0.00%
Ongoing: Participate in XSEDE communications plan	7/1/11	6/30/16	20.00%
Prototype NSFv4 wide area file system and investigate security implications	1/1/13	6/17/13	0.00%
Data Services	10/6/10	7/2/15	50.00%

Name	Start	Finish	% Completed - XSEDE
XSEDE Wide File System	10/6/10	7/2/15	33.33%
Evaluate/Select global parallel file system(s)	7/4/11	6/28/12	100.00%
Deploy/extend global parallel file system(s)	10/6/10	10/4/11	0.00%
Ongoing: Maintain/extend global parallel file system(s)	7/2/12	7/2/15	0.00%
Evaluate and design archival replication framework	7/1/11	6/27/12	100.00%
XSEDENet Networking	10/6/10	7/1/16	46.59%
Transition current TG network to XSEDE network	4/1/11	7/29/11	100.00%
Execute NLR contracts	4/1/11	7/1/11	100.00%
Connect XSEDE sites to NLR	6/27/11	7/29/11	100.00%
xsede.org nameservice	5/9/11	7/29/11	100.00%
delegate subdomains to XSEDE partners: NICS, TACC, PSC	5/9/11	7/29/11	100.00%
establish DNS entries for non-subdomain names (network.xsede.org, etc.)	5/9/11	7/29/11	100.00%
Ongoing: Maintain and Monitor XSEDEnet	7/29/11	6/30/16	20.00%
Preserve the PSC speed page	5/9/11	7/29/11	100.00%
Ongoing: Tune end-to-end performance for user applications	7/1/11	6/30/16	20.00%
Ongoing: Develop and implement improvements based on SEMP Spiral Design	7/1/11	6/30/16	20.00%
Setup perfSONAR	7/1/11	7/13/12	100.00%
Provide Operations tools to monitor the network	8/1/11	3/30/12	100.00%
Replace network.teragrid.org functions	8/1/11	3/30/12	100.00%
Evaluate alternatives to NLR	3/1/12	7/18/12	100.00%
Execute network vendor contracts	10/6/10	11/30/10	0.00%
Ongoing: Maintain DNS entries for non-subdomain names (network.xsede.org,	1/3/11	6/30/16	20.00%
Ongoing: Maintain perfSONAR	10/6/10	9/23/14	5.00%
Ongoing: Maintain Operations tools to monitor the network	10/6/10	1/5/15	20.00%
Ongoing: Develop/Implement special ops team process for network related application	7/2/12	7/1/16	0.00%
XSEDEnet Metrics	10/6/10	7/8/14	6.67%
Determine metrics	7/2/12	9/28/12	20.00%
Ongoing: Collect data	10/6/10	7/8/14	0.00%
Ongoing: Report metrics (dashboard, quarterly report)	10/6/10	7/8/14	0.00%

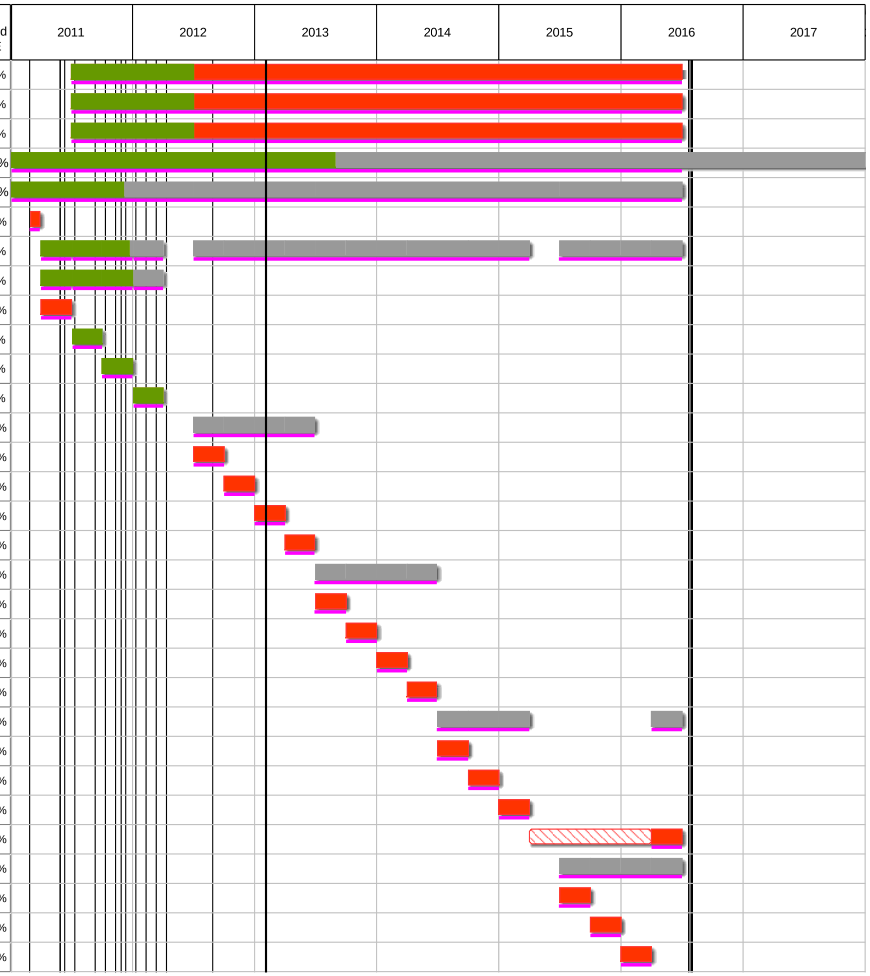
Name	Start	Finish	% Completed - XSEDE
SMNP Access, Layer 2 monitoring and measurement	7/2/12	7/1/16	0.00%
Develop Application Standards for Network Performance Metrics	7/2/12	7/1/16	0.00%
Software Testing and Deployment	10/6/10	6/30/16	45.38%
Test XSEDE software	7/4/11	11/29/12	100.00%
Test Grid Middleware - EMS (Unicore and Genesis II client)	7/4/11	11/29/12	100.00%
Test Grid Middleware - GFSS (Genesis II)	7/4/11	11/29/12	100.00%
Test Data Movement - Globus Online	7/4/11	11/29/12	100.00%
Deploy XSEDE software	10/6/10	10/26/12	50.00%
Deploy Grid Middleware - Unicore	10/6/10	5/3/11	50.00%
Deploy Grid Middleware - Genesis II (campus bridging)	10/6/10	5/3/11	50.00%
Deploy Grid Middleware - Globus Online	4/2/12	10/26/12	50.00%
Ongoing: Coordinate operational reviews of next increment of XSEDE software on	7/1/11	6/30/16	20.00%
Ongoing: Test next increment of XSEDE Software on demand	7/4/11	6/30/16	20.00%
Ongoing: Deploy next increment of XSEDE software to SPs on demand	7/4/11	6/30/16	20.00%
Ongoing: Coordinate campus bridging deployments	7/4/11	6/30/16	20.00%
Ongoing: Develop deployment work plans and documentation	7/4/11	6/30/16	20.00%
Ongoing: Coordinate Globus Grid software support	7/4/11	6/30/16	20.00%
Ongoing: Support Deployment of Software & Services at SPs	10/6/10	6/30/16	20.00%
Accounting and Account Management	5/9/11	7/1/16	34.44%
Ongoing: Maintain existing accounting and account management databases	7/1/11	6/30/16	20.00%
Ongoing: Investigate and improve accounting/account management processes	7/1/11	6/30/16	20.00%
Ongoing: Participate in XSEDE communications plan	7/1/11	6/30/16	20.00%
Optimize and upgrade the XDCDB system	7/1/11	3/29/12	100.00%
Ongoing: Develop and implement improvements based on SEMP Spiral Design	7/1/11	6/30/16	20.00%
Make appropriate name changes to {item}.xsede.org	5/9/11	7/29/11	100.00%
domain name changes	5/9/11	7/29/11	100.00%
web site changes	5/9/11	7/29/11	100.00%
documentation changes	5/9/11	7/29/11	100.00%
Complete the 2nd phase of vetted/unvetted account creation effort	5/9/11	3/30/12	100.00%
Ongoing: Maintain and enhance XSEDE-wide reporting, decision-support and	7/1/11	7/1/16	20.00%
Streamline and modernize the allocation-request and account	7/2/12	7/1/13	0.00%

2011 2012 2013 2014 2015 2016 2017

Name	Start	Finish	% Completed - XSEDE
Re-work and simplify the proposal submission process	7/2/12	6/28/13	0.00%
Improve the proposal review and approval process	1/1/13	7/1/13	0.00%
Provide enhanced A&AM administrative capabilties	1/1/13	7/1/13	0.00%
Streamline account-request process	7/2/12	1/4/13	0.00%
Enhance user-based information delivery (allocation/usage info, etc.)	7/2/12	10/5/12	0.00%
Improve overall A&AM-related documentation and training	7/2/12	1/11/13	0.00%
Establish processes to improve campus bridging and new SP integration	7/2/12	10/5/12	0.00%
Ongoing: Support hardware/infrastructure integrity (server maintenace, UPS, etc.)	7/1/11	6/30/16	20.00%
System Operational Support	10/6/10	6/30/16	62.05%
Setup XSEDE Operations Center	6/1/11	6/28/11	100.00%
Ongoing: Operate XSEDE Operations Center	7/1/11	6/30/16	20.00%
Deploy centralized XSEDE cyberinfrasture servers/services	5/30/11	8/31/12	75.00%
Ongoing: Maintain centralized XSEDE cyberinfrastructure servers/services	10/6/10	8/5/14	20.00%
Upgrade XDCDB hardware and split database and AMIE parts	5/9/11	8/12/11	100.00%
upgrade hardware at SDSC and operating system at PSC	5/9/11	8/12/11	100.00%
migrate AMIE to stand alone VM server (PSC and SDSC)	5/9/11	6/17/11	100.00%
Evaluate XDCDB hardware at PSC and determine if refresh needed	5/9/11	6/29/12	100.00%
Evaluate current TG services and classify them into XSEDE HA tiers	5/9/11	6/28/12	100.00%
Plan and schedule a semi-annual XDCDB failover test (SDSC to PSC)	5/9/11	6/28/12	100.00%
TeraGrid ticket system transition	7/1/11	8/11/11	100.00%
Evaluate/Deploy XSEDE Centralized monitoring software	11/1/11	6/21/13	100.00%
Participate in Ticket System evaluation in conjunction with User Support	7/1/11	2/2/12	100.00%
Transition Ticket System: Legacy to New	10/6/10	3/6/12	50.00%
Backup XOC setup at IU	11/1/11	6/28/13	0.00%
Documentation/Training for XOC Backup	11/1/11	6/28/13	0.00%
XOC Failover Test	11/1/11	6/28/13	0.00%
Operations Annual Report	10/6/10	6/28/12	100.00%
Prepare operational metrics annual report/internal Operational Assessment	6/1/12	6/28/12	100.00%
Milestone: Operational metrics annual report completed	10/6/10	10/6/10	100.00%
Ongoing: Participate in XSEDE communications plan	7/1/11	6/30/16	20.00%
Ongoing: Provide VM support for Centralized Services	7/1/11	6/30/16	20.00%



Name	Start	Finish	% Completed - XSEDE
Ongoing: Provide VM support for Science Gateway services	7/1/11	6/30/16	20.00%
Ongoing: Maintain VM server hardware	7/1/11	6/30/16	20.00%
Ongoing: Maintain other server hardware	7/1/11	6/30/16	20.00%
User Services	1/3/11	7/9/21	25.23%
Training	1/3/11	6/30/16	16.80%
Milestone: Develop guidelines for online and in-person training materials across XSEDE	3/1/11	3/28/11	0.00%
Milestone: Develop 10 Training Modules Annually	4/1/11	6/30/16	15.00%
Milestone: Develop 10 Training Modules Year 1	4/1/11	3/30/12	75.00%
Develop and Post 2 new online training tutorials	4/1/11	7/1/11	0.00%
Develop and Post 2 new online training tutorials	7/5/11	9/29/11	100.00%
Develop and Post 3 new online training tutorials	10/3/11	12/30/11	100.00%
Develop and Post 3 new online training tutorials	1/4/12	3/30/12	100.00%
Milestone: Develop 10 Training Modules Year 2	7/2/12	6/28/13	0.00%
Develop and Post 2 new online training tutorials	7/2/12	9/28/12	0.00%
Develop and Post 2 new online training tutorials	10/1/12	12/31/12	0.00%
Develop and Post 3 new online training tutorials	1/1/13	3/29/13	0.00%
Develop and Post 3 new online training tutorials	4/1/13	6/28/13	0.00%
Milestone: Develop 10 Training Modules Year 3	7/1/13	6/30/14	0.00%
Develop and Post 2 new online training tutorials	7/1/13	9/30/13	0.00%
Develop and Post 2 new online training tutorials	10/1/13	12/31/13	0.00%
Develop and Post 3 new online training tutorials	1/1/14	3/31/14	0.00%
Develop and Post 3 new online training tutorials	4/1/14	6/30/14	0.00%
Milestone: Develop 10 Training Modules Year 4	7/1/14	6/30/16	0.00%
Develop and Post 2 new online training tutorials	7/1/14	9/30/14	0.00%
Develop and Post 2 new online training tutorials	10/1/14	12/31/14	0.00%
Develop and Post 3 new online training tutorials	1/1/15	3/31/15	0.00%
Develop and Post 3 new online training tutorials	4/1/16	6/30/16	0.00%
Milestone: Develop 10 Training Modules Year 5	7/1/15	6/30/16	0.00%
Develop and Post 2 new online training tutorials	7/1/15	9/30/15	0.00%
Develop and Post 2 new online training tutorials	10/1/15	12/31/15	0.00%
Develop and Post 3 new online training tutorials	1/1/16	3/31/16	0.00%



Name	Start	Finish	% Completed - XSEDE
Develop and Post 3 new online training tutorials	4/1/16	6/30/16	0.00%
Conduct 50 Training Sessions Annually	4/1/11	6/30/16	18.75%
Milestone: Conduct 50 Training sessions Year 1	4/1/11	3/30/12	93.75%
Conduct first 10 in-person or webcast training sessions	4/1/11	7/1/11	100.00%
Conduct first 15 in-person or webcast training sessions	7/5/11	12/30/11	100.00%
Conduct first 10 in-person or webcast training sessions	10/3/11	12/30/11	75.00%
Conduct first 15 in-person or webcast training sessions	1/4/12	3/30/12	100.00%
Milestone: Conduct 50 Training sessions Year 2	7/2/12	6/28/13	0.00%
Conduct first 10 in-person or webcast training sessions	7/2/12	9/28/12	0.00%
Conduct first 15 in-person or webcast training sessions	10/1/12	12/31/12	0.00%
Conduct first 10 in-person or webcast training sessions	1/1/13	3/29/13	0.00%
Conduct first 15 in-person or webcast training sessions	4/1/13	6/28/13	0.00%
Milestone: Conduct 50 Training sessions Year 3	7/1/13	6/30/14	0.00%
Conduct first 10 in-person or webcast training sessions	7/1/13	9/30/13	0.00%
Conduct first 15 in-person or webcast training sessions	10/1/13	12/31/13	0.00%
Conduct first 10 in-person or webcast training sessions	1/1/14	3/28/14	0.00%
Conduct first 15 in-person or webcast training sessions	4/1/14	6/30/14	0.00%
Milestone: Conduct 50 Training sessions Year 4	7/1/14	6/30/15	0.00%
Conduct first 10 in-person or webcast training sessions	7/1/14	9/30/14	0.00%
Conduct first 15 in-person or webcast training sessions	10/1/14	12/31/14	0.00%
Conduct first 10 in-person or webcast training sessions	1/1/15	3/31/15	0.00%
Conduct first 15 in-person or webcast training sessions	4/1/15	6/30/15	0.00%
Milestone: Conduct 50 Training sessions Year 5	7/1/15	6/30/16	0.00%
Conduct first 10 in-person or webcast training sessions	7/1/15	9/30/15	0.00%
Conduct first 15 in-person or webcast training sessions	10/1/15	12/31/15	0.00%
Conduct first 10 in-person or webcast training sessions	1/1/16	3/31/16	0.00%
Conduct first 15 in-person or webcast training sessions	4/1/16	6/30/16	0.00%
Milestone: Complete Federation of existing online training materials with XSEDE	1/3/11	12/30/11	0.00%
Milestone: Complete 2 targeted community workshops annually	7/1/11	6/30/16	20.00%

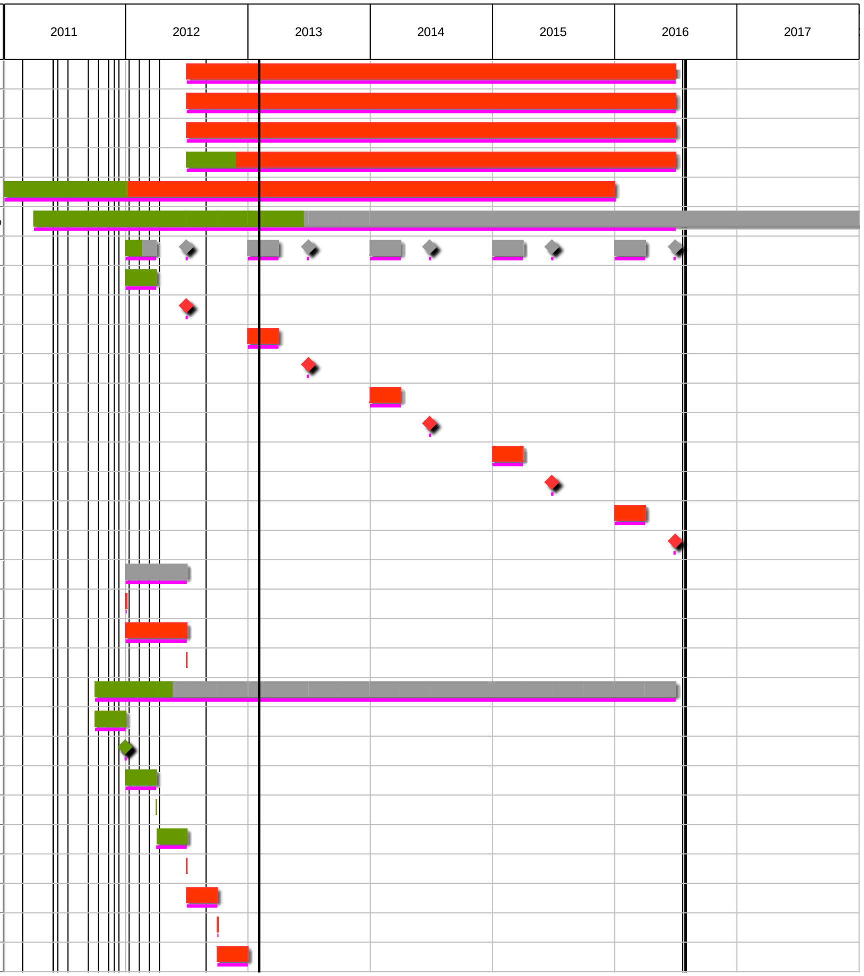
Name	Start	Finish	% Completed - XSEDE
Conduct first targeted community workshop Year 1	7/1/11	12/30/11	100.00%
Conduct second targeted community workshop Year 1	1/2/12	6/29/12	100.00%
Conduct first targeted community workshop Year 2	7/2/12	12/31/12	0.00%
Conduct second targeted community workshop Year 2	1/1/13	6/28/13	0.00%
Conduct first targeted community workshop Year 3	7/1/13	12/31/13	0.00%
Conduct second targeted community workshop Year 3	1/1/14	6/2/14	0.00%
Conduct first targeted community workshop Year 4	7/1/14	12/31/14	0.00%
Conduct second targeted community workshop Year 4	1/1/15	6/30/15	0.00%
Conduct first targeted community workshop Year 5	7/1/15	12/31/15	0.00%
Conduct second targeted community workshop Year 5	1/1/16	6/30/16	0.00%
Milestone: Conduct 4 technical training, content-based and mentoring webinars in	7/1/11	6/30/16	20.00%
Conduct 4 webinars in support of XSEDE Scholars Program Year 1	7/1/11	6/29/12	100.00%
Conduct 4 webinars in support of XSEDE Scholars Program Year 2	7/2/12	6/28/13	0.00%
Conduct 4 webinars in support of XSEDE Scholars Program Year 3	7/2/13	6/30/14	0.00%
Conduct 4 webinars in support of XSEDE Scholars Program Year 4	7/1/14	6/30/15	0.00%
Conduct 4 webinars in support of XSEDE Scholars Program Year 5	7/1/15	6/30/16	0.00%
Portfolio Review	1/3/11	1/3/11	100.00%
Focus areas	1/3/11	12/30/11	0.00%
Support of new systems (Stampede, Gordon, Keeneland, Blue Waters)	1/3/11	7/4/11	0.00%
XSEDE architecture and tools	1/3/11	12/30/11	0.00%
Security	1/3/11	7/4/11	0.00%
Train the trainers	1/3/11	7/4/11	0.00%
Trainiing for non-traditional areas	1/3/11	12/30/11	0.00%
Portal to API for gateways	7/2/12	6/28/13	0.00%
User Information Resources	1/3/11	6/30/16	47.31%
Milestone: Release Production User Portal & Web Site	4/1/11	7/1/11	100.00%
Transition existing production portal capabilities and web site	4/1/11	7/1/11	100.00%
Define user information architecture	4/1/11	6/23/11	100.00%
Milestone: Maintain Production User News System	4/1/11	7/1/11	100.00%
Transition existing user news system to production	4/1/11	7/1/11	100.00%
Milestone: Release Allocation & User Guide for New and Transitioning Users	4/1/11	10/11/11	100.00%

XSEDE

Name	Start	Finish	% Completed - XSEDE	2011	2012	2013	2014	2015	2016	2017
Document instructions for new users coming to XSEDE	4/1/11	7/1/11	100.00%							
Document instructions for existing users	7/4/11	9/5/11	100.00%							
Document allocation policies for resources	9/6/11	10/11/11	100.00%							
Milestone: Release new user guide with user comment capabilities	4/1/11	7/1/11	100.00%							
Create user guide template for HPC, Viz, Storage, etc.	4/1/11	6/23/11	100.00%							
Create user guide examples for each resource type	4/1/11	6/23/11	100.00%							
Ensure all user guides have been transitioned to template	4/1/11	7/1/11	100.00%							
Publish all user guides across web presence	4/1/11	7/1/11	100.00%							
Milestone: Production mobile user portal	4/1/11	6/30/11	66.67%							
Transition existing mobile framework	4/1/11	4/28/11	100.00%							
Evaluate requirements for mobile features	4/29/11	6/22/11	50.00%							
Create schedule for releasing future mobile features	4/29/11	6/30/11	50.00%							
Milestone: Release updated user news	7/1/11	9/22/11	100.00%							
Define requirements for user news system	7/1/11	7/28/11	100.00%							
Evaluate existing and alternative technologies	7/29/11	8/11/11	100.00%							
Release new user news system (if appropriate)	8/12/11	9/22/11	100.00%							
Milestone: Create new social media presence for XD	10/3/11	9/26/13	12.50%							
Define requirements for social media	10/3/11	9/3/12	50.00%							
Evaluate requirements that come out of User Engagement	10/31/11	9/26/13	0.00%							
Create twitter and facebook presence for users of XD and specifically XUP	7/2/12	12/31/12	0.00%							
Display twitter feeds on user portal	7/2/12	12/31/12	0.00%							
Milestone: Release collaborative capabilities to user portal	7/2/12	12/31/12	0.00%							
Define requirements based on User Engagement feedback	7/2/12	12/31/12	0.00%							
Enable users to be able to share calendars, chat, files, etc. with	7/2/12	12/31/12	0.00%							
Milestone: Release integrated training system	1/2/12	3/23/12	100.00%							
Define requirements for integrated training system based on TEOS and	1/2/12	1/27/12	100.00%							
Enable sites to post training courses on user portal	1/30/12	3/23/12	100.00%							
Enable sites to add online training resources to user portal	1/30/12	3/23/12	100.00%							
Enable users to register for training online via user portal	1/30/12	3/23/12	100.00%							
Create one stop shop for user training on user portal with calendar, SMS	1/30/12	3/23/12	100.00%							
Resource Selector	1/3/11	9/2/11	11.00%							

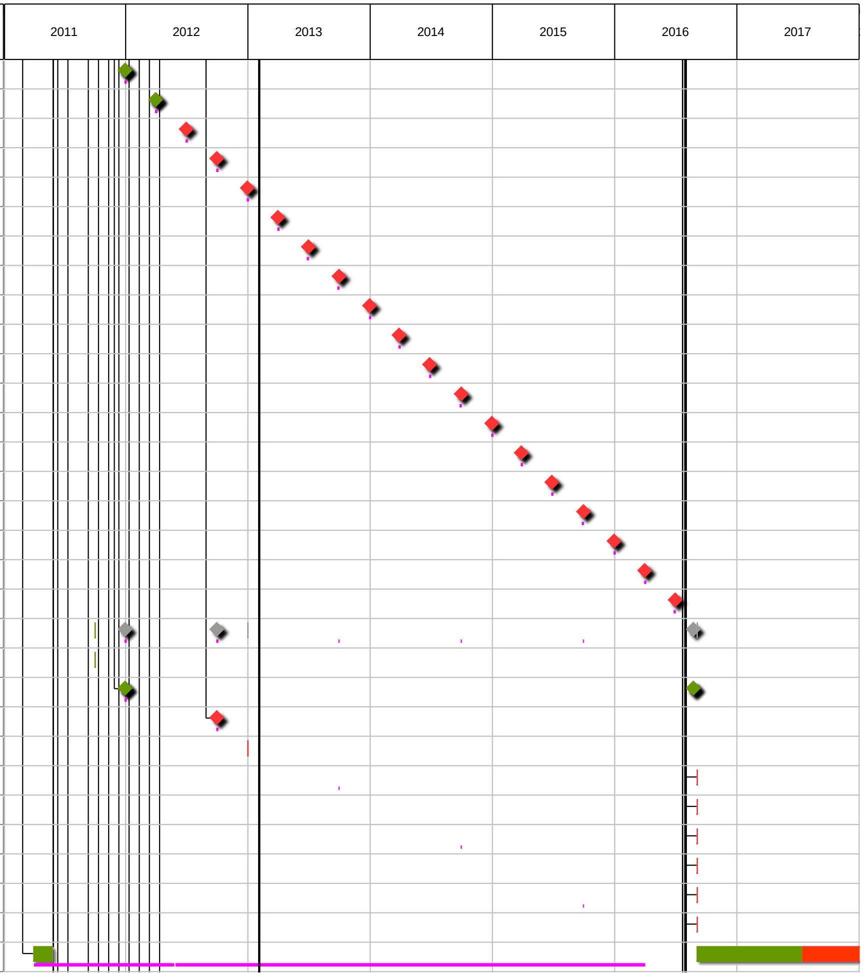
Name	Start	Finish	% Completed - XSEDE
Ongoing: Develop and implement improvements based on SEMP Spiral Design	1/3/11	6/30/16	25.65%
XSEDE User Portal	1/3/11	6/30/16	25.82%
Redesign dock at the top and apply theme	1/2/12	3/2/12	100.00%
Update profile portlet - expand with picture, publications,etc.	1/2/12	6/29/12	100.00%
Link checker for XUP & XSEDE web site	1/2/12	3/30/12	0.00%
Add forget username feature	1/2/12	4/30/12	100.00%
Integrate future grid status in XUP system monitor	1/2/12	6/29/12	0.00%
Expand system status beyond up/down/etc.	1/2/12	6/29/12	0.00%
Implement new News categories	1/2/12	3/30/12	100.00%
GridShib/InCommon integration	1/2/12	9/28/12	0.00%
Enable dynamic feedback on each page	1/2/12	3/30/12	100.00%
Migrate TGU staff queries to XUP staff area	1/2/12	3/30/12	75.00%
Compete guest homepage redesign	1/2/12	6/29/12	0.00%
Disable/gray out login link when resources are down	4/2/12	6/29/12	0.00%
Merge add/remove user page and allocation page	7/2/12	6/30/16	0.00%
Look at giving gateways a different 'view' for their community allocations	7/2/12	6/30/16	0.00%
Merge DN listing with user profile	7/2/12	6/30/16	0.00%
Integrate new ticketing system	7/2/12	12/31/12	0.00%
Chat for help	7/2/12	6/30/16	0.00%
Make hot links/bookmarking feature	7/2/12	6/30/16	0.00%
Screen sharing with support staff	7/2/12	6/30/16	0.00%
Expand allocations/usage/job history with graphs	7/2/12	6/30/16	100.00%
Integrate XDMoD services	7/2/12	6/30/16	9.00%
Custom views for communities: campus champions, gateways, fields	1/3/11	1/1/15	8.00%
Network connectivity monitor	7/2/12	6/30/16	0.00%
Dynamic visualization information in system monitor	7/2/12	6/30/16	0.00%
Remote visualization services	7/2/12	6/30/16	0.00%
RSS feeds and SMS notifications for user portal functions	7/2/12	6/30/16	50.00%
OSG documentation integration	7/2/12	6/30/16	100.00%
Videos & interactive guide on features of XUP	7/2/12	6/30/16	0.00%
Online training for XUP	7/2/12	6/30/16	0.00%

Name	Start	Finish	% Completed - XSEDE
Online survey for users on features	7/2/12	6/30/16	0.00%
Workflow management interface	7/2/12	6/30/16	0.00%
Metascheduling, job reservations, and ensemble job submission	7/2/12	6/30/16	0.00%
Change community account form to enter information in XCDB and	7/2/12	6/30/16	10.00%
Ongoing: Prioritize and integrate SD&I configuration items in US UII	1/3/11	12/31/15	20.00%
User Engagement	4/1/11	7/9/21	21.39%
Annual User Surveys	1/2/12	6/30/16	10.00%
Develop and Implement Y1 Annual User Survey	1/2/12	3/30/12	100.00%
Milestone: Y1 Annual User Survey report	7/2/12	7/2/12	0.00%
Develop and Implement Y2 Annual User Survey	1/1/13	4/1/13	0.00%
Milestone: Y2 Annual User Survey report	7/1/13	7/1/13	0.00%
Develop and Implement Y3 Annual User Survey	1/1/14	3/31/14	0.00%
Milestone: Y3 Annual User Survey report	6/30/14	6/30/14	0.00%
Develop and Implement Y4 Annual User Survey	1/1/15	3/31/15	0.00%
Milestone: Y4 Annual User Survey report	6/30/15	6/30/15	0.00%
Develop and Implement Y5 Annual User Survey	1/1/16	3/31/16	0.00%
Milestone: Y5 Annual User Survey report	6/30/16	6/30/16	0.00%
XSEDE CRM	1/2/12	7/2/12	0.00%
Document current XSEDE activities athat act as CRM	1/2/12	1/2/12	0.00%
Design and Implemnt initial CRM system	1/2/12	6/29/12	0.00%
Milestone: Initial CRM system deployed	7/2/12	7/2/12	0.00%
Data Mining	10/3/11	7/1/16	13.16%
Q1Y1 Data mining operations	10/3/11	12/30/11	100.00%
Milestone: Q1Y1 Data mining report	12/30/11	12/30/11	100.00%
Q2Y1 Data mining operations	1/2/12	3/30/12	100.00%
Milestone: Q2Y1 Data mining report	4/2/12	4/2/12	100.00%
Q3Y1 Data mining operations	4/3/12	7/2/12	100.00%
Milestone: Q3Y1 Data mining report	7/2/12	7/2/12	0.00%
Q4Y1 Data mining operations	7/3/12	10/1/12	0.00%
Milestone: Q4Y1 Data mining report	10/2/12	10/2/12	0.00%
Q1Y2 Data mining operations	10/2/12	12/31/12	0.00%



Name	Start	Finish	% Completed - XSEDE	2011	2012	2013	2014	2015	2016	2017
Milestone: Q1Y2 Data mining report	1/1/13	1/1/13	0.00%							
Q2Y2 Data mining operations	1/2/13	4/2/13	0.00%							
Milestone: Q2Y2 Data mining report	4/2/13	4/2/13	0.00%							
Q3Y2 Data mining operations	4/1/13	6/28/13	0.00%							
Milestone: Q3Y2 Data mining report	7/1/13	7/1/13	0.00%							
Q4Y2 Data mining operations	7/1/13	9/30/13	0.00%							
Milestone: Q4Y2 Data mining report	10/1/13	10/1/13	0.00%							
Q1Y3 Data mining operations	10/1/13	12/31/13	0.00%							
Milestone: Q1Y3 Data mining report	1/1/14	1/1/14	0.00%							
Q2Y3 Data mining operations	1/1/14	3/31/14	0.00%							
Milestone: Q2Y3 Data mining report	4/1/14	4/1/14	0.00%							
Q3Y3 Data mining operations	4/1/14	6/30/14	0.00%							
Milestone: Q3Y3 Data mining report	7/1/14	7/1/14	0.00%							
Q4Y3 Data mining operations	7/1/14	9/30/14	0.00%							
Milestone: Q4Y3 Data mining report	10/1/14	10/1/14	0.00%							
Q1Y4 Data mining operations	10/1/14	12/31/14	0.00%							
Milestone: Q1Y4 Data mining report	1/1/15	1/1/15	0.00%							
Q2Y4 Data mining operations	1/1/15	3/31/15	0.00%							
Milestone: Q2Y4 Data mining report	4/1/15	4/1/15	0.00%							
Q3Y4 Data mining operations	4/1/15	6/30/15	0.00%							
Milestone: Q3Y4 Data mining report	7/1/15	7/1/15	0.00%							
Q4Y4 Data mining operations	7/1/15	9/30/15	0.00%							
Milestone: Q4Y4 Data mining report	10/1/15	10/1/15	0.00%							
Q1Y5 Data mining operations	10/1/15	12/31/15	0.00%							
Milestone: Q1Y5 Data mining report	1/1/16	1/1/16	0.00%							
Q2Y5 Data mining operations	1/1/16	3/31/16	0.00%							
Milestone: Q2Y5 Data mining report	4/1/16	4/1/16	0.00%							
Q3Y5 Data mining operations	4/1/16	6/30/16	0.00%							
Milestone: Q3Y5 Data mining report	7/1/16	7/1/16	0.00%							
Develop Focus Group Topics and conduct focus groups	9/30/11	6/30/16	15.00%							
Milestone: Q1Y1 Focus Group Report	9/30/11	9/30/11	100.00%							

Name	Start	Finish	% Completed - XSEDE
Milestone: Q2Y1 Focus Group Report	1/2/12	1/2/12	100.00%
Milestone: Q3Y1 Focus Group Report	4/2/12	4/2/12	100.00%
Milestone: Q4Y1 Focus Group Report	7/2/12	7/2/12	0.00%
Milestone: Q1Y2 Focus Group Report	10/1/12	10/1/12	0.00%
Milestone: Q2Y2 Focus Group Report	12/31/12	12/31/12	0.00%
Milestone: Q3Y2 Focus Group Report	4/1/13	4/1/13	0.00%
Milestone: Q4Y2 Focus Group Report	7/1/13	7/1/13	0.00%
Milestone: Q1Y3 Focus Group Report	9/30/13	9/30/13	0.00%
Milestone: Q2Y3 Focus Group Report	12/31/13	12/31/13	0.00%
Milestone: Q3Y3 Focus Group Report	3/31/14	3/31/14	0.00%
Milestone: Q4Y3 Focus Group Report	6/30/14	6/30/14	0.00%
Milestone: Q1Y4 Focus Group Report	9/30/14	9/30/14	0.00%
Milestone: Q2Y4 Focus Group Report	12/31/14	12/31/14	0.00%
Milestone: Q3Y4 Focus Group Report	3/31/15	3/31/15	0.00%
Milestone: Q4Y4 Focus Group Report	6/30/15	6/30/15	0.00%
Milestone: Q1Y5 Focus Group Report	9/30/15	9/30/15	0.00%
Milestone: Q2Y5 Focus Group Report	12/31/15	12/31/15	0.00%
Milestone: Q3Y5 Focus Group Report	3/31/16	3/31/16	0.00%
Milestone: Q4Y5 Focus Group Report	6/30/16	6/30/16	0.00%
Develop and Conduct BoF Sessions	9/30/11	9/2/16	20.00%
Milestone: Conduct Y1 XSEDE BoF and Report	9/30/11	9/30/11	100.00%
Milestone: Conduct Y1 SC BoF and Report	1/2/12	8/25/16	100.00%
Milestone: Conduct Y2 XSEDE BoF and Report	9/30/12	10/1/12	0.00%
Milestone: Conduct Y2 SC BoF and Report	12/31/12	12/31/12	0.00%
Milestone: Conduct Y3 XSEDE BoF and Report	9/2/16	9/2/16	0.00%
Milestone: Conduct Y3 SC BoF and Report	9/2/16	9/2/16	0.00%
Milestone: Conduct Y4 XSEDE BoF and Report	9/2/16	9/2/16	0.00%
Milestone: Conduct Y4 SC BoF and Report	9/2/16	9/2/16	0.00%
Milestone: Conduct Y5 XSEDE BoF and Report	9/2/16	9/2/16	0.00%
Milestone: Conduct Y5 SC BoF and Report	9/2/16	9/2/16	0.00%
Conduct Usability Panels and Testing (as needed)	4/1/11	7/9/21	20.00%



Name	Start	Finish	% Completed - XSEDE	2011	2012	2013	2014	2015	2016	2017
User Engagement General Operations	7/1/11	9/3/20	20.00%							
Monitor tickets	7/1/11	9/3/20	20.00%							
Resolve XSEDE wide tickets	7/1/11	9/3/20	20.00%							
Bi-weekly User Engagement status meetings	7/1/11	9/3/20	20.00%							
Quarterly reporting	7/1/11	9/3/20	20.00%							
XSEDE Ticket System	4/1/11	4/29/13	45.45%							
Transition existing TG ticket system to production in XSEDE	4/1/11	4/27/12	100.00%							
Milestone: Release Production Ticketing System	7/7/11	4/29/13	100.00%							
Deploy new/improved XSEDE Ticket System	7/1/11	10/29/12	33.33%							
Define requirements for ticket system	7/1/11	8/31/12	100.00%							
Evaluate candidate ticket systems	8/15/11	10/29/12	100.00%							
Milestone: Select new/improved ticket system	10/3/11	8/31/12	100.00%							
Develop and deploy new/improved ticket system	10/3/11	3/30/12	0.00%							
Milestone: Release new/improved ticket system	3/31/12	4/2/12	0.00%							
Integrate new/improved ticket system with CRM	4/2/12	6/29/12	0.00%							
Milestone: Release Integrated CRM interface	6/29/12	6/29/12	0.00%							
Integrate new/improved ticket system with XSEDE User Portal	4/2/12	6/29/12	0.00%							
Milestone: Release Integrated XUP interface	6/29/12	6/29/12	0.00%							
Consulting Policies	10/3/11	5/31/16	25.00%							
Create consulting policies, procedures, and support guide	10/3/11	5/31/16	50.00%							
Milestone: Deploy consulting policies, procedures, and support guide	1/30/14	1/30/14	0.00%							
Contact PI at allocation start	7/15/11	11/17/17	28.57%							
Contact "new"/"renewal" PIs at the beginning of each XRAC allocation	7/15/11	11/17/17	100.00%							
Contact "new"/"renewal" PIs at the beginning of each XRAC allocation	7/15/11	1/30/14	100.00%							
Contact "new"/"renewal" PIs at the beginning of each XRAC allocation	10/17/11	1/30/14	100.00%							
Contact "new"/"renewal" PIs at the beginning of each XRAC allocation	1/16/12	1/30/14	100.00%							
Contact "new"/"renewal" PIs at the beginning of each XRAC allocation	4/16/12	4/28/15	100.00%							
Contact "new"/"renewal" PIs at the beginning of each XRAC allocation	4/29/15	4/29/15	100.00%							
Contact "new"/"renewal" PIs at the beginning of each XRAC allocation	9/1/15	9/1/15	0.00%							
Contact "new"/"renewal" PIs at the beginning of each XRAC allocation	1/30/14	1/30/14	0.00%							
Contact "new"/"renewal" PIs at the beginning of each XRAC allocation	10/29/15	10/29/15	0.00%							

Name	Start	Finish	% Completed - XSEDE
Contact "new"/"renewal" PIs at the beginning of each XRAC allocation	1/30/14	1/30/14	0.00%
Contact "new"/"renewal" PIs at the beginning of each XRAC allocation	1/29/16	1/29/16	0.00%
Contact "new"/"renewal" PIs at the beginning of each XRAC allocation	1/30/14	1/30/14	0.00%
Contact "new"/"renewal" PIs at the beginning of each XRAC allocation	4/29/16	4/29/16	0.00%
Contact "new"/"renewal" PIs at the beginning of each XRAC allocation	7/15/14	7/15/14	0.00%
Contact "new"/"renewal" PIs at the beginning of each XRAC allocation	10/15/14	10/15/14	0.00%
Contact "new"/"renewal" PIs at the beginning of each XRAC allocation	1/15/15	1/15/15	0.00%
Contact "new"/"renewal" PIs at the beginning of each XRAC allocation	4/15/15	4/15/15	0.00%
Contact "new"/"renewal" PIs at the beginning of each XRAC allocation	7/15/15	7/15/15	0.00%
Contact "new"/"renewal" PIs at the beginning of each XRAC allocation	10/15/15	10/15/15	0.00%
Contact "new"/"renewal" PIs at the beginning of each XRAC allocation	1/15/16	1/15/16	0.00%
Contact "new"/"renewal" PIs at the beginning of each XRAC allocation	4/15/16	4/15/16	0.00%
Contact "startup" PIs each month	7/15/11	9/2/16	25.00%
1	7/15/11	9/1/16	100.00%
2	8/15/11	9/1/16	100.00%
3	9/15/11	9/16/11	100.00%
4	10/17/11	9/2/16	100.00%
5	11/15/11	9/2/16	100.00%
6	12/15/11	9/2/16	100.00%
7	1/16/12	9/2/16	100.00%
8	2/15/12	9/2/16	100.00%
9	3/15/12	9/2/16	100.00%
10	4/16/12	9/2/16	100.00%
11	5/15/12	9/2/16	100.00%
12	9/2/16	9/2/16	100.00%
13	9/2/16	9/2/16	100.00%
14	8/15/12	8/15/12	100.00%
15	9/17/12	9/17/12	100.00%
16	10/15/12	10/15/12	0.00%
17	11/15/12	11/15/12	0.00%
18	4/29/13	4/29/13	0.00%

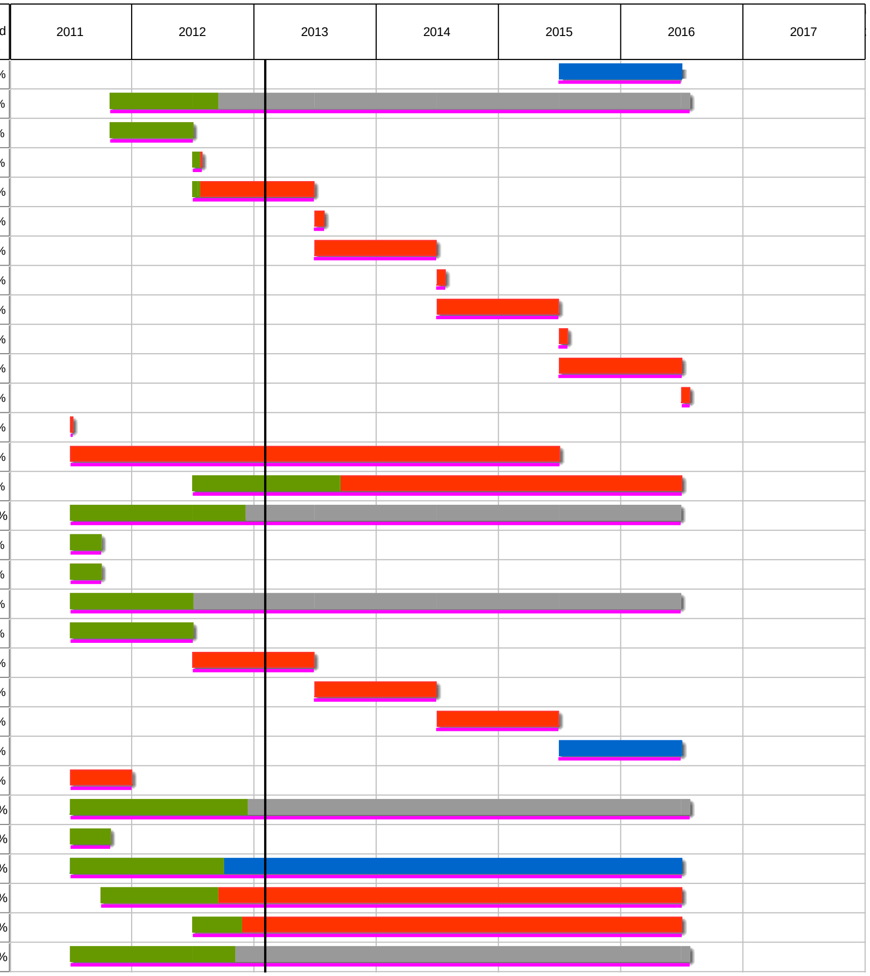
Name	Start	Finish	% Completed - XSEDE	2011	2012	2013	2014	2015	2016	2017
19	1/15/13	1/15/13	0.00%							
20	2/15/13	2/15/13	0.00%							
21	3/15/13	3/15/13	0.00%							
22	4/15/13	4/15/13	0.00%							
23	5/15/13	5/15/13	0.00%							
24	6/17/13	6/17/13	0.00%							
25	8/25/16	8/25/16	0.00%							
26	8/31/16	8/31/16	0.00%							
27	9/16/13	9/16/13	0.00%							
28	9/2/16	9/2/16	0.00%							
29	9/2/16	9/2/16	0.00%							
30	9/2/16	9/2/16	0.00%							
31	9/2/16	9/2/16	0.00%							
32	9/2/16	9/2/16	0.00%							
33	9/2/16	9/2/16	0.00%							
34	9/2/16	9/2/16	0.00%							
35	9/2/16	9/2/16	0.00%							
36	9/2/16	9/2/16	0.00%							
37	9/2/16	9/2/16	0.00%							
38	8/15/14	8/15/14	0.00%							
39	9/15/14	9/15/14	0.00%							
40	10/15/14	10/15/14	0.00%							
41	11/17/14	11/17/14	0.00%							
42	12/15/14	12/15/14	0.00%							
43	1/15/15	1/15/15	0.00%							
44	2/16/15	2/16/15	0.00%							
45	3/16/15	3/16/15	0.00%							
46	4/15/15	4/15/15	0.00%							
47	5/15/15	5/15/15	0.00%							
48	6/15/15	6/15/15	0.00%							
49	8/25/16	8/25/16	0.00%							

Name	Start	Finish	% Completed - XSEDE	2011	2012	2013	2014	2015	2016	2017
50	8/31/16	8/31/16	0.00%							
51	9/15/15	9/15/15	0.00%							
52	9/2/16	9/2/16	0.00%							
53	9/2/16	9/2/16	0.00%							
54	9/2/16	9/2/16	0.00%							
55	9/2/16	9/2/16	0.00%							
56	9/2/16	9/2/16	0.00%							
57	9/2/16	9/2/16	0.00%							
58	9/2/16	9/2/16	0.00%							
59	9/2/16	9/2/16	0.00%							
60	9/2/16	9/2/16	0.00%							
Allocations	1/3/11	9/2/16	22.45%							
Allocations policy in place	4/1/11	9/2/16	100.00%							
Host Quarterly Allocations Meetings Annually	9/1/11	9/2/16	31.25%							
Host Year 1 Quarterly Allocations Meetings	9/1/11	9/2/16	100.00%							
Host Quarterly Allocations Meeting	9/1/11	9/2/16	100.00%							
Host Quarterly Allocations Meeting	12/1/11	9/2/16	100.00%							
Host Quarterly Allocations Meeting	3/1/12	9/2/16	100.00%							
Host Quarterly Allocations Meeting	9/2/16	9/2/16	100.00%							
Host Year 2 Quarterly Allocations Meetings	9/2/16	9/2/16	25.00%							
Host Quarterly Allocations Meeting	9/2/16	9/2/16	100.00%							
Host Quarterly Allocations Meeting	9/2/16	9/2/16	0.00%							
Host Quarterly Allocations Meeting	9/2/16	9/2/16	0.00%							
Host Quarterly Allocations Meeting	9/2/16	9/2/16	0.00%							
Host Year 3 Quarterly Allocations Meetings	9/2/16	9/2/16	0.00%							
Host Quarterly Allocations Meeting	9/2/16	9/2/16	0.00%							
Host Quarterly Allocations Meeting	9/2/16	9/2/16	0.00%							
Host Quarterly Allocations Meeting	9/2/16	9/2/16	0.00%							
Host Quarterly Allocations Meeting	9/2/16	9/2/16	0.00%							
Host Year 4 Quarterly Allocations Meetings	9/2/16	9/2/16	0.00%							
Host Quarterly Allocations Meeting	9/2/16	9/2/16	0.00%							

Name	Start	Finish	% Completed - XSEDE	2011	2012	2013	2014	2015	2016	2017
Host Quarterly Allocations Meeting	9/2/16	9/2/16	0.00%							
Host Quarterly Allocations Meeting	9/2/16	9/2/16	0.00%							
Host Quarterly Allocations Meeting	9/2/16	9/2/16	0.00%							
Conduct How to Write a Successful Proposal Webcasts Annually	1/3/11	9/2/16	25.00%							
Conduct Year 1 How to Write a Successful Proposal Webcast	8/1/11	9/2/16	100.00%							
Conduct How to Write a Successful Proposal Webcast	8/1/11	9/2/16	100.00%							
Conduct How to Write a Successful Proposal Webcast	11/1/11	9/2/16	100.00%							
Conduct How to Write a Successful Proposal Webcast	2/1/12	9/2/16	100.00%							
Conduct How to Write a Successful Proposal Webcast	5/1/12	9/2/16	100.00%							
Conduct Year 2 How to Write a Successful Proposal Webcast	9/2/16	9/2/16	25.00%							
Conduct How to Write a Successful Proposal Webcast	9/2/16	9/2/16	100.00%							
Conduct How to Write a Successful Proposal Webcast	9/2/16	9/2/16	0.00%							
Conduct How to Write a Successful Proposal Webcast	9/2/16	9/2/16	0.00%							
Conduct How to Write a Successful Proposal Webcast	9/2/16	9/2/16	0.00%							
Conduct Year 3 How to Write a Successful Proposal Webcast	1/3/11	9/2/16	0.00%							
Conduct How to Write a Successful Proposal Webcast	9/2/16	9/2/16	0.00%							
Conduct How to Write a Successful Proposal Webcast	9/2/16	9/2/16	0.00%							
Conduct How to Write a Successful Proposal Webcast	9/2/16	9/2/16	0.00%							
Conduct How to Write a Successful Proposal Webcast	1/3/11	1/3/11	0.00%							
Conduct Year 4 How to Write a Successful Proposal Webcast	9/2/16	9/2/16	0.00%							
Conduct How to Write a Successful Proposal Webcast	9/2/16	9/2/16	0.00%							
Conduct How to Write a Successful Proposal Webcast	9/2/16	9/2/16	0.00%							
Conduct How to Write a Successful Proposal Webcast	9/2/16	9/2/16	0.00%							
Conduct How to Write a Successful Proposal Webcast	9/2/16	9/2/16	0.00%							
Conduct Year 5 How to Write a Successful Proposal Webcast	9/2/16	9/2/16	0.00%							
Conduct How to Write a Successful Proposal Webcast	9/2/16	9/2/16	0.00%							
Conduct How to Write a Successful Proposal Webcast	9/2/16	9/2/16	0.00%							
Conduct How to Write a Successful Proposal Webcast	9/2/16	9/2/16	0.00%							
Conduct How to Write a Successful Proposal Webcast	9/2/16	9/2/16	0.00%							
New POPS Interface	2/13/12	9/2/16	0.00%							
Design new interface	2/13/12	4/2/12	0.00%							

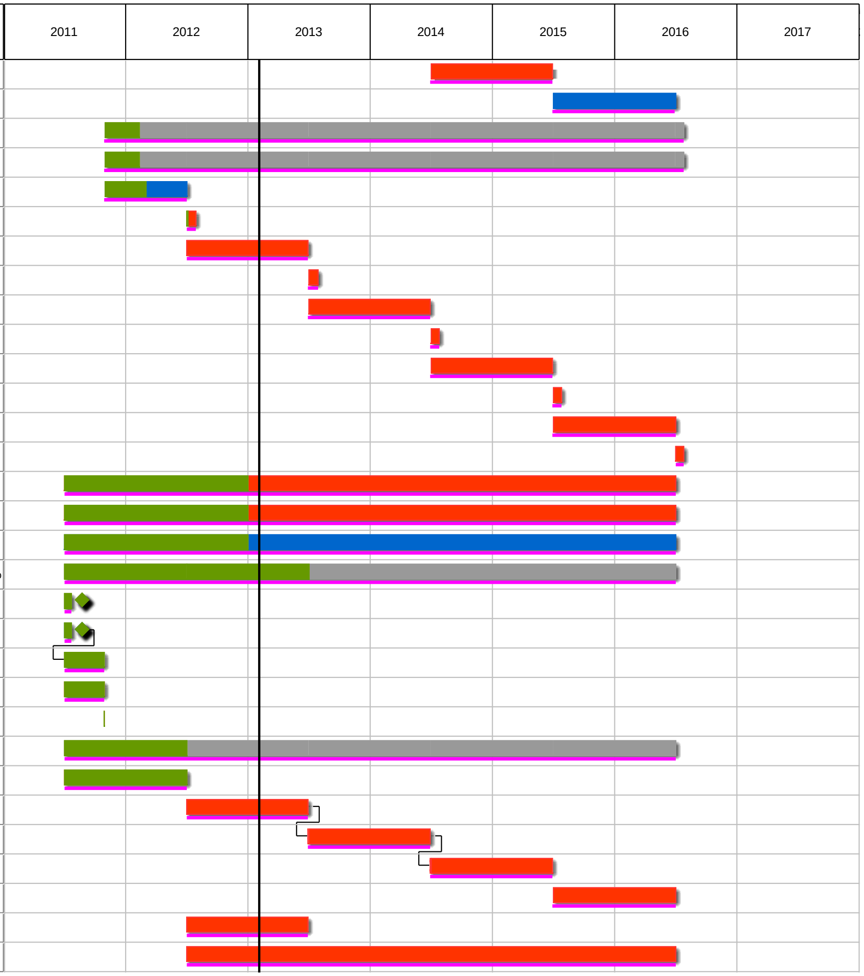
Name	Start	Finish	% Completed - XSEDE
Implement and test	4/2/12	6/29/12	0.00%
Deploy	9/2/16	9/2/16	0.00%
Add Tier 2 resources to allocation process	1/3/11	12/30/11	0.00%
Implement Allocation Levels and Types	1/3/11	6/28/13	0.00%
Levels	7/2/12	6/28/13	0.00%
Small	7/2/12	6/28/13	0.00%
Standard	7/2/12	6/28/13	0.00%
XRAC	7/2/12	6/28/13	0.00%
Types	1/3/11	6/28/13	0.00%
Storage	1/3/11	12/30/11	0.00%
Visualization	7/2/12	6/28/13	0.00%
Throughput	7/2/12	6/28/13	0.00%
Advanced Support for Research Teams (ECSS)	7/2/12	6/28/13	0.00%
GPU, MIC, other non-heterogeneous x86 compute	7/2/12	6/28/13	0.00%
Extended Collaborative Support Service (ECSS)-Projects	7/1/11	7/22/16	33.13%
Create/ test proj. mgmt. framework for ECSS work plans/reporting	7/1/11	10/28/11	100.00%
Add at least 1 external FTE to fill an identified skills gap	7/1/11	6/30/16	100.00%
Fill 1.5 Discretionary Hires (as needed)	7/2/12	6/28/13	33.33%
Host monthly symposium open to ECSS, XSEDE staff, and Users	10/3/11	6/30/16	20.00%
Conduct continuing training of ECSS Staff as needed	7/2/12	6/30/16	20.00%
Extended Support for Research Team (ESRT)	7/1/11	7/22/16	29.52%
Establish ESRT group	7/1/11	7/21/11	100.00%
Set up ESRT staff and management teams and communications	7/1/11	7/21/11	100.00%
Milestone: Support 20 ESRT Projects Annually	7/1/11	7/22/16	28.82%
Work w/TG AUS to transition ASTA Projs. To ESRT mgmt.	7/1/11	10/28/11	100.00%
Milestone: All TG ASTA proj. managed as XD ESRT Projs.	10/28/11	10/28/11	100.00%
Work with XD CMS to Generate 20 new XD ESRT projs. Annually	7/1/11	6/30/16	21.00%
Year 1 Generate 20 new XD ESRT projects	7/1/11	6/29/12	100.00%
Year 2 Generate 20 new XD ESRT projects	7/2/12	6/28/13	5.00%
Year 3 Generate 20 new XD ESRT projects	7/1/13	6/30/14	0.00%
Year 4 Generate 20 new XD ESRT projects	7/1/14	6/30/15	0.00%

Name	Start	Finish	% Completed - XSEDE
Year 5 Generate 20 new XD ESRT projects	7/1/15	6/30/16	0.00%
20 ESRT work plans documented and actively managed annually	10/31/11	7/22/16	18.50%
Year 1 - 20 work plans documented	10/31/11	6/29/12	100.00%
milestone: Y1 prepare and complete Final Reports	7/2/12	7/27/12	80.00%
Year 2 - 20 work plans documented	7/2/12	6/28/13	5.00%
milestone: Y2 prepare and complete Final Reports	7/1/13	7/26/13	0.00%
Year 3 - 20 work plans documented	7/1/13	6/30/14	0.00%
milestone: Y3 prepare and complete Final Reports	7/1/14	7/25/14	0.00%
Year 4 - 20 work plans documented	7/1/14	6/30/15	0.00%
milestone: Y4 prepare and complete Final Reports	7/1/15	7/24/15	0.00%
Year 5 - 20 work plans documented	7/1/15	6/30/16	0.00%
milestone: Y5 prepare and complete Final Reports	7/1/16	7/22/16	0.00%
Organize and execute HPC workshop at IEEE E-Science conference	7/1/11	7/7/11	0.00%
Host Annual Workshop on Petascale Computing	7/1/11	7/1/15	0.00%
Conduct XRAC Meetings Adaptive Reviews	7/2/12	6/30/16	30.00%
Novel & Innovative Projects	7/1/11	6/29/16	28.57%
Establish NIP group	7/1/11	9/30/11	100.00%
Set up NIP staff and management teams and communications	7/1/11	9/30/11	100.00%
Milestone: Generate 20 new XSEDE+ ECS NIPs Annually	7/1/11	6/29/16	20.00%
Year 1-work w/XD CMS,TEOS,TIS to generate 20 XD NIP projects	7/1/11	6/29/12	100.00%
Year 2-work w/XD CMS,TEOS,TIS to generate 20 XD NIP projects	7/2/12	6/28/13	0.00%
Year 3-work w/XD CMS,TEOS,TIS to generate 20 XD NIP projects	7/1/13	6/30/14	0.00%
Year 4-work w/XD CMS,TEOS,TIS to generate 20 XD NIP projects	7/1/14	6/30/15	0.00%
Year 5-work w/XD CMS,TEOS,TIS to generate 20 XD NIP projects	7/1/15	6/29/16	0.00%
Milestone: Create ECSS Project work plans	7/1/11	12/30/11	0.00%
Extended Collaborative Support Service - Communities	7/1/11	7/22/16	28.61%
Create/ test proj. mgmt. framework for ESCC work plans/reporting	7/1/11	10/28/11	100.00%
Add at least 1 external FTE to fill an identified skills gap	7/1/11	6/30/16	25.00%
Host monthly symposium for ECSS and XSEDE staff	10/3/11	6/30/16	20.00%
Conduct Continuing Training of ECSS Staff as needed	7/2/12	6/30/16	10.00%
Extended Support for Community Codes (ESCC)	7/1/11	7/22/16	26.50%



Name	Start	Finish	% Completed - XSEDE	2011	2012	2013	2014	2015	2016	2017
Establish ESCC group	7/1/11	8/25/11	100.00%							
Set up ESCC staff and management teams and communications	7/1/11	8/25/11	100.00%							
Transition TG ASP proj. to ESCC management	7/1/11	10/28/11	100.00%							
Milestone:Active TG ASP proj. managed as XD ESCC proj.	10/28/11	10/28/11	100.00%							
Milestone: Support 10 ESCC Projects Annually	7/1/11	7/22/16	15.33%							
Year 1-Work w/TG CMS,TEOS,TIS to generate 10 XD ESCC proj.	7/1/11	6/29/12	100.00%							
Year 2-Work w/TG CMS,TEOS,TIS to generate 10 XD ESCC proj.	7/2/12	6/28/13	10.00%							
Year 3-Work w/TG CMS,TEOS,TIS to generate 10 XD ESCC proj.	7/1/13	6/30/14	0.00%							
Year 4-Work w/TG CMS,TEOS,TIS to generate 10 XD ESCC proj.	7/1/14	6/30/15	0.00%							
Year 5-Work w/TG CMS,TEOS,TIS to generate 10 XD ESCC proj.	7/1/15	6/30/16	0.00%							
Milestone: Create 10 ESCC work plans Annually	10/31/11	7/22/16	12.00%							
Y1 - 10 work plans documented	10/31/11	6/29/12	100.00%							
milestone: Y1 prepare and complete Final Reports	7/2/12	7/27/12	10.00%							
Y2 - 10 work plans documented	7/2/12	6/28/13	10.00%							
milestone: Y2 prepare and complete Final Reports	7/1/13	7/26/13	0.00%							
Y3 - 10 work plans documented	7/1/13	6/30/14	0.00%							
milestone: Y3 prepare and complete Final Reports	7/1/14	7/25/14	0.00%							
Y4 - 10 work plans documented	7/1/14	6/30/15	0.00%							
milestone: Y4 prepare and complete Final Reports	7/1/15	7/24/15	0.00%							
Y5 - 10 work plans documented	7/1/15	6/30/16	0.00%							
milestone: Y5 prepare and complete Final Reports	7/1/16	7/22/16	0.00%							
Work with the TIS group to evaluate and recommend SI2 software projects for	7/2/12	6/30/16	0.00%							
Develop documentation, sample scripts, optimized builds to cover the top community	7/2/12	6/30/16	0.00%							
Extended Collaborative Support Service - Science Gateways	7/1/11	7/22/16	23.00%							
Establish ESSGW group	7/1/11	6/30/16	100.00%							
Set up ESSGW staff and management teams and communications	7/1/11	8/25/11	100.00%							
Organize bi-weekly gateway community calls open to all XSEDE users	9/1/11	6/30/16	100.00%							
Milestone: Support 10 Science Gateways Annually	7/1/11	7/22/16	11.33%							
Year 1-Work w/TG CMS,TEOS,TIS to generate 10 XD ESSGW proj.	7/1/11	6/29/12	100.00%							
Year 2-Work w/TG CMS,TEOS,TIS to generate 10 XD ESSGW proj.	7/2/12	6/28/13	10.00%							
Year 3-Work w/TG CMS,TEOS,TIS to generate 10 XD ESSGW proj.	7/1/13	6/30/14	0.00%							

Name	Start	Finish	% Completed - XSEDE
Year 4-Work w/TG CMS,TEOS,TIS to generate 10 XD ESSGW proj.	7/1/14	6/30/15	0.00%
Year 5-Work w/TG CMS,TEOS,TIS to generate 10 XD ESSGW proj.	7/1/15	6/30/16	0.00%
Milestone: Create ESSGW work plans	10/31/11	7/22/16	6.00%
At least 10 ESSGW work plans documented&actively managed	10/31/11	7/22/16	6.00%
Y1 - 10 work plans documented	10/31/11	6/29/12	50.00%
milestone: Y1 prepare and complete Final Reports	7/2/12	7/27/12	10.00%
Y2 - 10 work plans documented	7/2/12	6/28/13	0.00%
milestone: Y2 prepare and complete Final Reports	7/1/13	7/26/13	0.00%
Y3 - 10 work plans documented	7/1/13	6/30/14	0.00%
milestone: Y3 prepare and complete Final Reports	7/1/14	7/25/14	0.00%
Y4 - 10 work plans documented	7/1/14	6/30/15	0.00%
milestone: Y4 prepare and complete Final Reports	7/1/15	7/24/15	0.00%
Y5 - 10 work plans documented	7/1/15	6/30/16	0.00%
milestone: Y5 prepare and complete Final Reports	7/1/16	7/22/16	0.00%
Gateway Outreach: Constantly reach out to new potential gateways independently and	7/1/11	6/30/16	30.00%
XSEDE Requirements: Work with Gateway community in analyzing the XSEDE	7/1/11	6/30/16	30.00%
XSEDE Architecture Test Cases: Provide Test Cases to SD&I teams in nature of tests	7/1/11	6/30/16	30.00%
Extended Support for Training Education and Outreach (ESTEO)	7/1/11	6/30/16	40.00%
Establish ESTEO group	7/1/11	8/25/11	100.00%
Set up ESTEO staff and management teams and communications	7/1/11	8/25/11	100.00%
Milestone: Contribute content for TEO modules	7/1/11	10/28/11	100.00%
Work w/TG AUS to transition ASEOT projs. to XD ESTEO mgmt.	7/1/11	10/28/11	100.00%
Milestone: All TG ASEOT projs. Managed as XD ESTEO projs.	10/28/11	10/28/11	100.00%
Milestone: 50 ESTEO projects/activities supported Annually	7/1/11	6/30/16	20.00%
Year 1-work w/XD CMS, TEOS, TIS to generate 50 XD ESTEO	7/1/11	6/29/12	100.00%
Year 2- work w/XD CMS, TEOS, TIS to generate 50 XD ESTEO	7/2/12	6/28/13	0.00%
Year 3 - work w/XD CMS, TEOS, TIS to generate 50 XD ESTEO	7/1/13	6/30/14	0.00%
Year 4 - work w/XD CMS, TEOS, TIS to generate 50 XD ESTEO	7/1/14	6/30/15	0.00%
Year 5 - work w/XD CMS, TEOS, TIS to generate 50 XD ESTEO	7/1/15	6/30/16	0.00%
Test and Document initial work assignments for UCB CS class using XSEDE resouces	7/2/12	6/28/13	0.00%
Arrange ECSS Internal Training Seminars Annually	7/2/12	6/30/16	0.00%



Name	Start	Finish	% Completed - XSEDE	2011	2012	2013	2014	2015	2016	2017
Education and Outreach	4/4/11	7/1/13	46.54%							
Education	7/1/11	7/1/13	66.25%							
Milestone: 2 HPC Graduate level summer schools annually	7/1/11	6/28/13	75.00%							
Milestone: 2 HPC Graduate level summer schools annually	7/1/11	10/3/11	100.00%							
Milestone: 2 HPC Graduate level summer schools annually	7/2/12	6/28/13	50.00%							
Milestone: 5 summer workshops annually	7/1/11	7/1/13	55.00%							
Milestone: 5 summer workshops annually	7/1/11	10/3/11	100.00%							
Milestone: 5 summer workshops annually	7/2/12	7/1/13	10.00%							
Milestone: Add certificate programs at specific universities	7/1/11	7/1/13	60.00%							
Milestone: ID univ to work with to dev vert pgm	7/1/11	12/30/11	100.00%							
Milestone:Add cert and/or deg pgm @ univ and cont to ID univs for cert pgm	7/2/12	7/1/13	20.00%							
Milestone: Provide online educational services	7/1/11	6/28/13	75.00%							
Milestone: Provide online educational services	7/1/11	10/3/11	100.00%							
Milestone: Provide online educational services	7/2/12	6/28/13	50.00%							
Outreach	6/1/11	7/1/13	72.86%							
Underrepresented Engagement	7/1/11	7/1/13	75.00%							
Milestone: 10 campus visits (SURA)	7/1/11	6/28/13	75.00%							
Milestone: 10 campus visits (SURA)	7/1/11	10/3/11	100.00%							
Milestone: 10 campus visits (SURA)	7/2/12	6/28/13	50.00%							
Milestone: Engage 40 underrepresented individuals (Rice)	7/1/11	6/28/13	75.00%							
Milestone: Engage 40 underrepresented individuals (Rice)	7/1/11	10/3/11	100.00%							
Milestone: Engage 40 underrepresented individuals (Rice)	7/2/12	6/28/13	50.00%							
Milestone: Create Faculty Council with 20 minority faculty (Rice)	7/1/11	7/1/13	75.00%							
Milestone: Create Faculty Council with 20 minority faculty (Rice)	7/1/11	12/30/11	100.00%							
Milestone: Create Faculty Council with 20 minority faculty (Rice)	7/2/12	7/1/13	50.00%							
Speakers' Bureau	7/1/11	6/28/13	75.00%							
Milestone: 10 National/Regional presentations	7/1/11	6/28/13	75.00%							
Milestone: 10 National/Regional presentations	7/1/11	10/3/11	100.00%							
Milestone: 10 National/Regional presentations	7/2/12	6/28/13	50.00%							
Student Engagement	7/1/11	6/28/13	60.00%							
Milestone: Recruit 20 students for training/mentoring/internship	7/1/11	6/28/13	60.00%							

Name	Start	Finish	% Completed - XSEDE	2011	2012	2013	2014	2015	2016	2017
Milestone: Recruit 20 students for training/mentoring/internship	7/1/11	10/3/11	100.00%							
Milestone: Recruit 20 students for training/mentoring/internship	7/2/12	6/28/13	20.00%							
Campus Champions	7/1/11	6/28/13	75.00%							
Milestone: Increase impact in Campus Champions program	7/1/11	6/28/13	75.00%							
Milestone: Increase membership in Campus Champions program	7/1/11	10/3/11	100.00%							
Milestone: Increase impact in Campus Champions program	7/2/12	6/28/13	50.00%							
XSEDE Annual Conference	6/1/11	6/28/13	75.00%							
XSEDE 12	6/1/11	10/3/11	100.00%							
XSEDE 13	7/2/12	6/28/13	50.00%							
Community Requirements	4/4/11	6/28/13	75.00%							
TEOS Advisory Committee	4/4/11	6/28/13	75.00%							
Semi-Annual consultation with TEOS Advisory Group	4/4/11	11/16/11	100.00%							
TEOS Advisory Committee	7/2/12	6/28/13	50.00%							
Collect Community Requirements	4/4/11	6/28/13	75.00%							
Annual collection and analysis of community needs and requirements	4/4/11	11/16/11	100.00%							
Collect Community Requirements	7/2/12	6/28/13	50.00%							
Infratructure	4/4/11	6/28/13	66.67%							
Curation of TEOS information on public web and XSEDE portal	4/4/11	10/3/11	100.00%							
E&O Curation	7/2/12	6/28/13	50.00%							
E&O Infrastructure Lead	7/2/12	6/28/13	50.00%							
Campus Bridging	4/4/11	6/28/13	10.48%							
Lead Campus Bridging Effort	4/4/11	6/28/13	36.67%							
Ongoing: Share information with campuses interested in campus bridging	4/4/11	10/3/11	100.00%							
Lead Campus Bridging Effort	7/2/12	6/28/13	50.00%							
Campus Bridging Travel to Pilot Program Sites(Task replaced 1/23/13)	7/2/12	6/28/13	0.00%							
Pilot program, software packaging, documentation and suppport (Task	7/2/12	6/28/13	50.00%							
Rocks Roll test cluster 10GbE at Cornell(Task replaced 1/23/13)	7/2/12	6/28/13	10.00%							
Rocks Roll test cluster Infiniband at IU(Task Replaced 1/23/13)	7/2/12	6/28/13	10.00%							
Pilot program	2/1/12	4/30/13	0.00%							
Pilot site preparatory meetings	2/1/12	12/31/12	0.00%							
Operations deployment plan for beta grid	7/2/12	12/28/12	0.00%							

Name	Start	Finish	% Completed - XSEDE	2011	2012	2013	2014	2015	2016	2017
XSEDE beta grid in place	8/1/12	3/29/13	0.00%							
XSEDE GFFS Container Software installed at SP's	1/1/13	3/29/13	0.00%							
XSEDE GFFS Software installers ready for pilot sites	12/3/12	2/1/13	0.00%							
Pilot sites using GFFS Software	1/1/13	3/28/13	0.00%							
Pilot metrics and case studies created	2/1/13	4/30/13	0.00%							
Evaluation discussions with pilots	2/1/13	4/30/13	0.00%							
Software packaging program	12/3/12	6/28/13	0.00%							
Software package list	12/3/12	2/28/13	0.00%							
Rocks roll for XSEDE-like cluster	1/1/13	2/28/13	0.00%							
Rocks testing by Operations	3/1/13	5/31/13	0.00%							
Cobbler/Puppet configuration scripts/recipes	2/1/13	4/30/13	0.00%							
RPMs for XSEDE software packages	3/1/13	3/29/13	0.00%							
RPM testing by Operations	4/1/13	6/28/13	0.00%							
Software distribution site & channels	3/1/13	3/29/13	0.00%							
External Evaluation	4/4/11	6/28/13	75.00%							
External Evaluator Quarterly Reports	4/4/11	10/3/11	100.00%							
External Evaluation	7/2/12	6/28/13	50.00%							
Technology Investigation Service	6/1/12	12/30/15	17.61%							
Technology Identification	7/2/12	8/2/13	44.44%							
Plan and Execute TIS Merge	8/20/12	9/28/12	50.00%							
Create QA/Testing/backup plan	7/2/12	7/3/12	100.00%							
Identify ER content coordinator for new TIS site	7/2/12	7/3/12	100.00%							
Market TIS to Technologies	7/2/12	6/28/13	25.00%							
Market TIS to user	7/2/12	6/28/13	25.00%							
Plan for increased access to TIS - ex. In common Authentication	4/1/13	8/2/13	0.00%							
Enable users to add comments to technologies - such as likes and feedbacks	8/28/12	12/31/12	25.00%							
Enable evaluators to enter evaluations for multiple pieces of a single technology	7/2/12	9/21/12	50.00%							
Plan for future release iterations of XTED based on requirements	7/2/12	6/28/13	25.00%							
Technology Evaluation	6/1/12	12/30/15	10.71%							
Receive the requirements from other Level 3s.	10/1/12	9/27/13	25.00%							
Providing evaluation results to the XSEDE Level 3 implementers.	4/1/13	7/18/14	25.00%							

Name	Start	Finish	% Completed - XSEDE
Transfer Evaluation results to the Level 3 implementers.	4/1/13	3/28/14	25.00%
Transfer TIS knowledge and deployment objects to Level 3 implementers	7/22/13	7/18/14	25.00%
Make data available to other XSEDE Level 3s about the evaluation process, data	10/1/13	9/29/14	25.00%
Maintain/update system access accounts to XSEDE RP systems for TEP members	1/1/14	12/30/14	25.00%
Maintain Test hardware	7/21/14	9/29/15	25.00%
Maintain/administer TEP acquired hardware	7/21/14	7/17/15	25.00%
Maintenance/administration of the TEL dedicated hardware	10/1/14	9/29/15	25.00%
Update XTED as appropriate	1/1/15	12/30/15	25.00%
Accomplish multiple evaluations annually	6/1/12	11/11/15	1.56%
Evaluation 5: Pegasus WMS- finish	6/1/12	11/11/15	25.00%
Evaluation 6: Unicore WMS – finish	6/1/12	11/15/12	0.00%
Evaluation 7: GFFS Reliable File Transfer(Second Attempt) – start	7/2/12	8/2/12	0.00%
Evaluation 7: GFFS Reliable File Transfer(Second Attempt) – finish	7/2/12	8/2/12	0.00%
Evaluation 8: Safenet - start	10/15/12	11/15/12	0.00%
Evaluation 8: Safenet – finish	7/2/12	8/2/12	0.00%
Evaluation 9: DUO – start	7/2/12	8/2/12	0.00%
Evaluation 9: DUO – finish	7/2/12	8/2/12	0.00%
Evaluation 10: VIP – start	7/2/12	8/2/12	0.00%
Evaluation 10: VIP – finish	7/2/12	8/2/12	0.00%
Evaluation 11: unspecified candidate – start	7/2/12	8/2/12	0.00%
Evaluation 11: unspecified candidate – finish	7/2/12	8/2/12	0.00%
Evaluation 12: unspecified candidate – start	7/2/12	8/2/12	0.00%
Evaluation 12: unspecified candidate – finish	7/2/12	8/2/12	0.00%
Evaluation 13: unspecified candidate – start	7/2/12	8/2/12	0.00%
Evaluation 13: unspecified candidate – finish	7/2/12	8/2/12	0.00%
Verify the evaluation process annually	7/2/12	4/8/13	0.00%
review the evaluation process	4/1/13	4/8/13	0.00%
update the evaluation process post review as necessary	7/2/12	7/9/12	0.00%
Assist in updating the process to identify User Requirements and the next item for	7/23/12	7/19/13	25.00%
Maintain/update the TEP portion of the XSEDE wiki	7/23/12	7/19/13	25.00%
Documentation	7/23/12	4/12/13	33.33%

Name	Start	Finish	% Completed - XSEDE	2011	2012	2013	2014	2015	2016	2017
Document TEL Dedicated Hardware	7/23/12	8/3/12	100.00%							
Document FutureGrid systems	4/1/13	4/12/13	0.00%							
Provide short document for specific TIS activities for others	10/1/12	10/4/12	0.00%							
Create an evaluation process for hardware	4/1/13	5/24/13	0.00%							
Create a training package for new TEP members to orient them on the TEP process	10/15/12	11/15/12	0.00%							
Train new members with the training package	7/2/12	7/11/12	0.00%							
Virtual Machines	4/1/13	4/19/13	0.00%							
Create images that closely mirrors XSEDE SP systems	4/1/13	4/19/13	0.00%							

Gantt Legend

Project (Gantt Bar Styles)

Default	Completed	Scheduled	Baseline 1				

Task (Gantt Bar Styles)

Default	Completed	Scheduled	Free Float	Total Float	Negative Float	Start Delay	Baseline 1
Critical Filter	Scheduled						
Parent Filter	Scheduled						
Buffers	Scheduled						
Buffer Incursion 0% - 25%	Buffer Incursion						
Buffer Incursion 25% - 75%	Buffer Incursion						
Buffer Incursion 75% - 100%	Buffer Incursion						

Task (Gantt Symbols)

Default	Objective Start	Objective Finish	Gantt Baseline2 Finish	Gantt Baseline3 Finish	Gantt Baseline4 Finish	Gantt Baseline5 Finish

C XSEDE Risk Register

Home > Risks Register > XSEDE Risks Summary

Risks Summary

Risk Summary Stats	
Total Number of Risks:	133
Number of non-retired Risks:	101
High Impact Risks:	28
High Probability Risks:	10
High Risk-Level:	2
Key Risks:	1
Current Risks:	96
(stats count non-retired risks)	

All Risks (Probability × Impact)

1	8	3
16	32	22
17	12	22

Non-retired Risks (Probability × Impact)

1	7	2
16	27	9
11	11	17

Retired Risks (Probability × Impact)

	1	1
	5	13
6	1	5

Non-retired Risks

101 risks

Risk Id	Risk	Risk Level	Probability	Impact	Status	Subproject	Monitor Date	Retire Da
273	Grid Software Scaling	High	High	High	Monitor	1.1.3 Architecture & Design	Apr 01, 2011	Mar 31, 2016
272	Grid Software System Integration	High	High	High	Monitor	1.1.3 Architecture & Design	Apr 01, 2011	Mar 31, 2016
350	Admins are not required to use strong authentication for management of XSEDE services.	High	High	Medium	Monitor	1.2.1 Security	Oct 22, 2012	Oct 22, 2016
328	Campus Bridging expectation management	High	High	Medium	Monitor	1.6.5 Campus Bridging	Oct 01, 2012	Dec 31, 2013
296	Capacity of XSEDE reources less than demand	High	Medium	High	Monitor	1.1 Project Office	Jul 01, 2011	Jun 30, 2016
278	Implementation delays and inconsistencies	High	High	Medium	Monitor	1.2.4 Software Testing & Deployment	Jul 01, 2011	Jul 01, 2016
369	Lack of Process to insure that the application and user cases/requirements are defined up front.	High	Medium	High	Monitor	1.7 TIS	Oct 30, 2012	Jun 30, 2015
287	Loss of Project PI or co-PI	High	Medium	High	Monitor	1 XSEDE	Jan 01, 2011	Jun 30, 2016

258	Mismatch between research teams' needs, XD resources, and AUSS staff availability.	High	Medium	High	Monitor	1.4 Extended Collaborative Support - Projects	Apr 01, 2011	Mar 31, 2016
312	Network Disruption Disables Critical Services	High	Medium	High	Monitor	1.2.3 XSEDEnet	Jul 01, 2011	Jul 01, 2015
301	Opportunity: Leverage new/novel resources	High	Medium	High	Monitor	1.1 Project Office	Jul 01, 2011	
331	Program Plan	High	Medium	High	Monitor	1.1.1 Project Management and Reporting	Feb 16, 2012	Jul 01, 2015
362	Security policies and procedures from TeraGrid are out-of-date	High	High	Medium	Monitor	1.2.1 Security	Oct 23, 2012	Oct 23, 2016
250	Suitable project management framework and process is not available.	High	Medium	High	Monitor	1.4.1 Extended Collaborative Research Teams Support	Jul 01, 2011	Mar 31, 2016
360	There is a zero-day root escalation exploit in the wild for Linux or some common piece of the XSEDE software stack	High	High	Medium	Monitor	1.2.1 Security	Oct 23, 2012	Oct 23, 2016
Risk Id	Risk	Risk Level	Probability	Impact	Status	Subproject	Monitor Date	Retire Da
364	There is no regular security training for users and service providers, and security policies lack visibility.	High	High	Medium	Monitor	1.2.1 Security	Oct 23, 2012	Oct 23, 2016
274	Usage of deployed software and services	High	High	Medium	Monitor	1.2.4 Software Testing & Deployment	Jul 01, 2011	Jul 01, 2016
298	XSEDE archival storage gap	High	Medium	High	Monitor	1.2.2 Data Services	Jul 01, 2011	Jun 30, 2016
343	Automated services may use unencrypted private keys to access XSEDE	Medium	Medium	Medium	Monitor	1.2.1 Security	Oct 22, 2012	Oct 22, 2016
252	Campus Infrastructure	Medium	Medium	Medium	Monitor	1.6.5 Campus Bridging	Jul 01, 2011	Mar 31, 2016
318	Communication Breakdown	Medium	Medium	Medium	Monitor	1.2.6 Systems Operational Support	Jul 01, 2011	Jul 01, 2016
371	Delay in "In-Common Authentication" availability	Medium	Medium	Medium	Monitor	1.7.1 Technology Identification	Oct 30, 2012	Mar 30, 2013
325	Delay in program implementation	Medium	Medium	Medium	Monitor	1.6.1 Education	Sep 19, 2011	Sep 30, 2012
356	Deployed software could be out of date, especially without coordinated patch manage-ment and stale CTSS registrations info	Medium	Medium	Medium	Monitor		Oct 23, 2012	Oct 23, 2016

305	Federated identity management does not catch on	Medium	Medium	Medium	Monitor	1.1 Project Office	Jul 01, 2011	Jun 30, 2014
363	Grand-fathered in services or software are exploited	Medium	Medium	Medium	Monitor	1.2.1 Security	Oct 23, 2012	Oct 23, 2016
365	Incident response resources at different SPs vary, and the XSEDE incident response (IR) team is geographically distributed.	Medium	Medium	Medium	Monitor	1.2.1 Security	Oct 23, 2012	Oct 23, 2016
347	Inconsistent or non-existent backup processes	Medium	Medium	Medium	Monitor		Oct 22, 2012	Oct 22, 2016
271	Insufficient Service Provider Integration into XSEDE activities	Medium	Medium	Medium	Monitor	1.1 Project Office	Jan 01, 2011	Mar 31, 2016
251	Mentoring Program	Medium	Medium	Medium	Monitor	1.6.2 Outreach	Jul 01, 2011	Mar 31, 2016
Risk Id	Risk	Risk Level	Probability	Impact	Status	Subproject	Monitor Date	Retire Da
352	No consistent patch management process for all XSEDE services and systems	Medium	Medium	Medium	Monitor	1.2.1 Security	Oct 23, 2012	Oct 23, 2016
373	Non-optimum arrival of tool evaluation requests.	Medium	Medium	Medium	Execute Contingency	1.7.2 Technology Evaluation	Oct 30, 2012	Jun 30, 2015
277	Noncompliant service provider	Medium	Medium	Medium	Monitor	1.1 Project Office	Apr 01, 2011	Mar 31, 2016
253	Remote User Support	Medium	Medium	Medium	Monitor	1.6.5 Campus Bridging	Jul 01, 2011	Mar 31, 2016
322	Suitable project management framework and process is not available	Medium	Medium	Medium	Monitor	1.5.2 Extended Collaborative Science Gateways Support	Jul 01, 2011	Mar 31, 2016
255	Suitable project management framework and process is not available.	Medium	Medium	Medium	Monitor	1.5.1 Extended Support for Community Codes	Jul 01, 2011	Mar 31, 2016
257	Suitable project management framework and process is not available.	Medium	Medium	Medium	Monitor	1.5.3 Extended Collaborative EOT Support	Jul 01, 2011	Mar 31, 2016
366	There are no security baselines for most services, and there is no regular auditing with respect to security	Medium	Medium	Medium	Monitor	1.2.1 Security	Oct 23, 2012	Oct 23, 2016
361	There is a common XSEDE service with a remote exploit	Medium	Medium	Medium	Monitor	1.2.1 Security	Oct 23, 2012	Oct 23, 2016
246	Training - Sync delivery	Medium	Medium	Medium	Monitor	1.3.1 Training	Jul 01, 2011	Mar 31, 2016

359	XSEDE depends upon software that is no longer actively supported	Medium	Medium	Medium	Monitor		Oct 23, 2012	Oct 23, 2016
346	XSEDE hardening guidelines for SPs are optional and unaudited	Medium	Medium	Medium	Monitor	1.2.1 Security	Oct 22, 2012	Oct 22, 2016
351	XSEDE has no centralized security monitoring	Medium	Medium	Medium	Monitor	1.2.1 Security	Oct 22, 2012	Oct 22, 2016
367	XSEDE has very complex organizational and procedural structures.	Medium	Medium	Medium	Monitor	1.2.1 Security	Oct 23, 2012	Oct 23, 2016
357	XSEDE relies heavily on in-house software that has not had code audits	Medium	Medium	Medium	Monitor	1.2.1 Security	Oct 23, 2012	Oct 23, 2016
Risk Id	Risk	Risk Level	Probability	Impact	Status	Subproject	Monitor Date	Retire Da
266	Architecture Obsolescence & Software Risks	Medium	Low	High	Monitor	1.1.2 Systems and Software Engineering	Apr 01, 2011	Mar 31, 2016
370	Dependencies on operational support for services from outside sources.	Medium	Low	High	Monitor	1.7 TIS	Oct 30, 2012	Jun 30, 2015
288	Differing architectural views hinder deployment and operation of XSEDE	Medium	Low	High	Monitor	1.1.2 Systems and Software Engineering	Mar 01, 2011	Jun 30, 2016
332	Failure of XDCDB failover process	Medium	Low	High	Monitor	1.2.6 Systems Operational Support	Jun 18, 2012	Jul 01, 2016
260	Failure of XSEDE Operational Infrastructure	Medium	Low	High	Monitor	1.2.6 Systems Operational Support	Jul 01, 2011	Jul 01, 2016
295	Funds are not provided for initial network "gap" costs	Medium	Low	High	Monitor	1.2.3 XSEDEnet	Jul 01, 2011	Jun 30, 2016
276	Inadequate communication with SPs	Medium	Low	High	Monitor	1.1 Project Office	Jan 01, 2011	Mar 31, 2016
372	LifeRay license expires without renewal.	Medium	Low	High	Monitor	1.7.1 Technology Identification	Oct 30, 2012	Jun 30, 2015
254	Mismatch between research teams' needs, XD resources, and ECSS staff availability.	Medium	Low	High	Monitor	1.5.1 Extended Support for Community Codes	Jul 01, 2011	Mar 31, 2016
256	Mismatch between research teams' needs, XD resources, and ECSS staff availability.	Medium	Low	High	Monitor	1.5.3 Extended Collaborative EOT Support	Jul 01, 2011	Mar 31, 2016
248	Mismatch maintained between research teams' needs, XD resources, and ECSS staff	Medium	Low	High	Monitor	1.4.1 Extended Collaborative Research Teams Support	Jul 01, 2011	Mar 31, 2016

	availability.							
311	NLR Services Are Inadequate	Medium	Low	High	Monitor	1.2.3 XSEDEnet	Jul 01, 2011	Jul 01, 2016
316	Prohibitive Cost for Required Software	Medium	Low	High	Monitor	1.2.4 Software Testing & Deployment	Jul 01, 2011	Jul 01, 2016
265	Technical Obsolesence	Medium	Low	High	Monitor	1.1.3 Architecture & Design	Apr 01, 2011	Mar 31, 2016
317	TeraGrid Domain Name Hardcoded into SP Software	Medium	High	Low	Monitor	1.2.6 Systems Operational Support	Jul 01, 2011	Jul 01, 2016
Risk Id	Risk	Risk Level	Probability	Impact	Status	Subproject	Monitor Date	Retire Da
242	XRAC Meeting Costs	Medium	Low	High	Monitor	1.3.4 Allocations	Jul 01, 2011	Mar 31, 2016
314	XSEDE DNS Service Availability	Medium	Low	High	Monitor	1.2.3 XSEDEnet	Jul 01, 2011	Jul 01, 2016
315	XSEDE RS Service Availability	Medium	Low	High	Monitor	1.2.3 XSEDEnet	Jul 01, 2011	Jul 01, 2015
334	Abuse of shared accounts	Low	Medium	Low	Monitor	1.2.1 Security	Oct 22, 2012	Oct 22, 2016
275	Deviation from project management procedures	Low	Medium	Low	Monitor	1.1.1 Project Management and Reporting	Jan 01, 2011	Mar 31, 2016
309	Genesis II FUSE/RNS scalability and performance	Low	Low	Medium	Monitor	1.2.2 Data Services	Jul 31, 2011	Oct 31, 2012
354	Helpdesk tickets are emailed in plaintext	Low	Medium	Low	Monitor	1.2.1 Security	Oct 23, 2012	Oct 23, 2016
338	Identity vetting procedures are abused or circumvented	Low	Medium	Low	Monitor	1.2.1 Security	Oct 22, 2012	Oct 22, 2016
335	Inconsistent authentication standards exploited to spread attacks	Low	Medium	Low	Monitor	1.2.1 Security	Oct 22, 2012	Oct 22, 2016
307	Integrating services fail to meet standards in service level agreements	Low	Medium	Low	Monitor	1.1 Project Office	Jul 01, 2011	Jun 30, 2016
330	Lack of Testing Resources	Low	Medium	Low	Monitor	1.2.4 Software Testing & Deployment	Jan 10, 2012	Jul 01, 2016
270	Loss of Senior Technical Personnel	Low	Low	Medium	Monitor	1 XSEDE	Apr 01, 2011	Mar 31, 2016
339	Mail list abuse	Low	Medium	Low	Monitor	1.2.1 Security	Oct 22, 2012	Oct 22, 2016
321	Mismatch between non-traditional users' needs, XSEDE services, and NIP staff allocation.	Low	Medium	Low	Monitor	1.4.2 Novel & Innovative Projects	Jul 01, 2011	Jun 30, 2016
326	NLR Business Focus Changes	Low	Low	Medium	Monitor	1.2.3 XSEDEnet	Sep 01, 2011	Jul 01, 2016
Risk Id	Risk	Risk Level	Probability	Impact	Status	Subproject	Monitor Date	Retire Da

327	Namespace collisions between XSEDE software and local software	Low	Medium	Low	Monitor	1.2.4 Software Testing & Deployment	Oct 03, 2011	Jul 01, 2016
333	Outdated Critical Documents	Low	Low	Medium	Monitor	1.2 XSEDE Operations	Aug 16, 2012	Jul 01, 2016
319	Overloading XSEDE Operations Center Staff	Low	Medium	Low	Monitor	1.2.6 Systems Operational Support	Jul 01, 2011	Jul 01, 2016
306	Plan for long term service scaling may not meet short term needs	Low	Medium	Low	Monitor	1.1 Project Office	Jul 01, 2011	Jun 30, 2016
239	Potential equipment failure can disrupt database services.	Low	Low	Medium	Monitor	1.2.5 Accounting/Account Mgmt	Jul 01, 2011	Jul 01, 2016
241	Prohibitive Operating Costs for Hardware or Software	Low	Low	Medium	Monitor	1.2.6 Systems Operational Support	Jul 01, 2011	Jul 01, 2016
368	Resources for security in XSEDE could be inadequate	Low	Medium	Low	Monitor	1.2.1 Security	Oct 23, 2012	Oct 23, 2016
341	Self-service password resets are abused	Low	Medium	Low	Monitor	1.2.1 Security	Oct 22, 2012	Oct 22, 2016
268	Software Partner Failure	Low	Low	Medium	Monitor	1.1.3 Architecture & Design	Apr 01, 2011	Mar 31, 2016
249	Student Internships	Low	Medium	Low	Monitor	1.6.2 Outreach	Jul 01, 2011	Mar 31, 2016
245	Training - AUSS support	Low	Low	Medium	Monitor	1.3.1 Training	Jul 01, 2011	Mar 31, 2016
261	UNICORE project is cancelled	Low	Low	Medium	Monitor	1.1.3 Architecture & Design	Jan 01, 2011	Mar 31, 2015
344	Uses may not adequately protect their private keys	Low	Medium	Low	Monitor	1.2.1 Security	Oct 22, 2012	Oct 22, 2016
244	XD Architecture not fully implemented at an XD Service Provider	Low	Low	Medium	Monitor	1.1 Project Office	Apr 01, 2011	Mar 31, 2016
262	XD Service Provider has insufficient resources to implement XSEDE Architecture	Low	Low	Medium	Monitor	1.2.4 Software Testing & Deployment	Jul 01, 2011	Jul 01, 2016
Risk Id	Risk	Risk Level	Probability	Impact	Status	Subproject	Monitor Date	Retire Da
340	Conference call system uses weak or loosely managed PINs	Low	Low	Low	Monitor		Oct 22, 2012	Oct 22, 2016
329	Delay in ticketing system interface release	Low	Low	Low	Monitor	1.3.2 User Information & Interfaces	Jan 01, 2012	Jan 01, 2013
247	Education Workshops	Low	Low	Low	Monitor	1.6.1 Education	May 01, 2011	Mar 31, 2016
345	Forensic trail is lost because of no centralized logging in XSEDE	Low	Low	Low	Monitor	1.2.1 Security	Oct 22, 2012	Oct 22, 2016

355	IR IM chats could be exposed without one's knowledge	Low	Low	Low	Monitor	1.2.1 Security	Oct 23, 2012	Oct 23, 2016
269	Lack of Qualified System Administration Personnel	Low	Low	Low	Monitor	1.1.2 Systems and Software Engineering	Mar 01, 2011	Mar 31, 2016
337	One-off authentication systems make account revocation more fragile	Low	Low	Low	Monitor	1.2.1 Security	Oct 22, 2012	Oct 22, 2012
267	Software Complexity	Low	Low	Low	Monitor	1.2.4 Software Testing & Deployment	Jul 01, 2011	Jul 01, 2016
358	Some XSEDE resources depend upon proprietary, unvetted protocols.	Low	Low	Low	Monitor		Oct 23, 2012	Oct 23, 2016
342	Unencrypted credentials are harvested for attacks	Low	Low	Low	Monitor	1.2.1 Security	Oct 22, 2012	Oct 22, 2016
353	User data has weak isolation guarantees on most resources	Low	Low	Low	Monitor	1.2.1 Security	Oct 23, 2012	Oct 23, 2016

Retired risks

Retired Risks

D XSEDE Change Control Report

Nothing to report this quarter.

E Metrics

To demonstrate its success and help focus management attention on areas in need of improvement, XSEDE monitors a wide range of metrics in support of different aspects of "success" for the program. The metrics presented in the quarterly reports provide a view into XSEDE's user community, including its success at expanding that community, the projects and allocations through which XSEDE manages access to resources, and the use of the resources by those projects (§E.1). In addition, XSEDE has identified metrics describing the program's success at delivering centralized services to this community, including operations, user support, advanced user support, and education and outreach activities (§E.2). Together, these metrics provide perspectives on how XSEDE works to ensure that the XSEDE-associated services and resources deliver science impact for the science and engineering research community.

E.1 XSEDE Resource and Service Usage Metrics

Table 15 highlights a few key XSEDE measures that summarize the user community, the projects and allocations, and resource utilization for Q4 2012. Notably, XSEDE saw a dip in open user accounts although the number of active individuals remained high, with 2,223 recording usage on SP systems. Gateways continued to represent a major part of the XSEDE community, with a new high of 1,629 users submitting jobs via science gateways. More user community details are in §E.1.1.

Table 15. Quarterly activity summary

User Community	**Q1 2012**	**Q2 2012**	**Q3 2012**	**Q4 2012**
Open user accounts	6,313	6,636	6,964	6,464
Active individuals	2,165	2,245	2,148	2,229
Gateway users	1,039	1,580	1,624	1,629
New user accounts	1,063	760	863	644
Active fields of science	26	29	29	31
Active institutions	340	375	354	357
Projects and Allocations				
NUs available at XRAC	17.377B	17.939B	22.429B	31.142B
NUs requested at XRAC	36.959B	37.539B	57.611B	71.429B
NUs recommended by XRAC	20.562B	23.194B	19.738B	37.963B
NUs awarded at XRAC	18.230B	17.502B	18.149B	29.820B
Open projects	1,545	1,600	1,612	1,606
Active projects	979	1,027	1,044	1,019
Active gateways	17	16	16	15
New projects	216	247	212	201
Closed projects	219	207	218	229
Resources and Usage				
Resources open (all types)	23	24	24	24
Total peak petaflops	2.92	2.92	3.54	3.39
Resources reporting use	14	13	14	13
Jobs reported	1.04M	1.70M	1.32M	1.62M
NUs delivered	14.76B	16.67B	17.9B	17.4B
Avg wtd run time (hrs)	23.3	20.9	22.4	23.4
Avg wtd wait time (hrs)	23.2	32.6	36.5	30.1
Avg wtd slow down	3.3	4.7	4.1	3.6

Project and allocation activity showed continued high demand, with XSEDE resources requested at 229% of what was available by 188 XRAC requests, an all-time high, despite a 40% increase in available resources for the coming quarter with the arrival of the TACC Stampede system. The XRAC recommendations, however, fit within the resources available. During the quarter, 1,606 open projects had access to resources, and 1,019 made use of the resources. More details are in §E.1.2.

XSEDE computing resources represented 3.4 Pflops (peak) at the end of the quarter, due to the NCSA Forge system ending production in the prior quarter; Stampede will increase the peak available as of Q1 2013. The central accounting system showed 13 resources reporting activity, and together they delivered 17.4 billion NUs of computing. This represents an decrease of approximately 3.5% over the previous quarter. At the same time, XSEDE users experienced slightly shorter wait times, response times, and slow downs, on average. More details are in §E.1.3.

E.1.1 User community metrics

Figure 43 shows the five-year trend in the XSEDE user community, including open user accounts, total active XSEDE users, active individual accounts, active gateway users, the number of new accounts, and the total number of unvetted user accounts (i.e., portal-only accounts) at the end of each quarter. Unvetted user accounts can be used for training course registration and other functions.

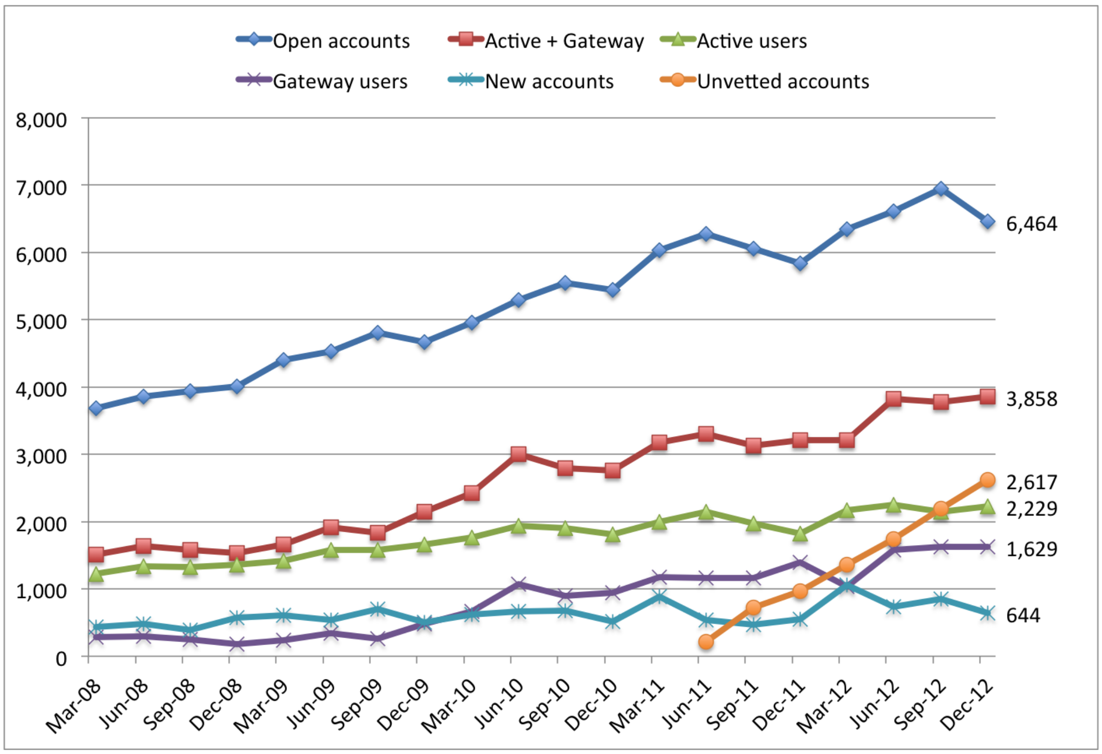


Figure 43. XSEDE user census, excluding XSEDE staff.

Figure 44 shows the activity on XSEDE resources according to field of science, including the relative fraction of PIs, open accounts, active users, allocations, and NUs used according to discipline. For consistency across quarters, we show the nine fields of science that typically consume ~2% or more of delivered NUs per quarter. PIs and users are counted more than once if they are associated with projects in different fields of science. The Q4 data show that the percentages of PIs and accounts associated with the "other" disciplines represent nearly 30% of all PIs, more than 30% of user accounts, and more than 25% of active users. Collectively the "other" fields of science represent 6.7% of total quarterly usage, led by activity in environmental biology and ocean sciences. Figure 45 shows the number of publications, conference papers, and presentations reported by XSEDE users each quarter, including the 1,112 reported by 122 projects in Q4; Appendix F lists these publications according to allocated project. The large increase in Q4 is likely explained, in part, by the number of requests at the XRAC meeting, which received 30 more requests than the prior quarter.

Table 16 and Table 17 highlight aspects of the broader impact of XSEDE. The former shows that graduate students, post-doctoral researchers, and undergraduates make up 65% of the XSEDE user base. The latter table shows XSEDE's reach into targeted institutional communities. Institutions with Campus Champions represent a large portion of XSEDE's usage because this table shows all users at Campus Champion institutions, not just those on the champion's project. The table also shows XSEDE's reach into EPSCoR states, the MSI community, and internationally.

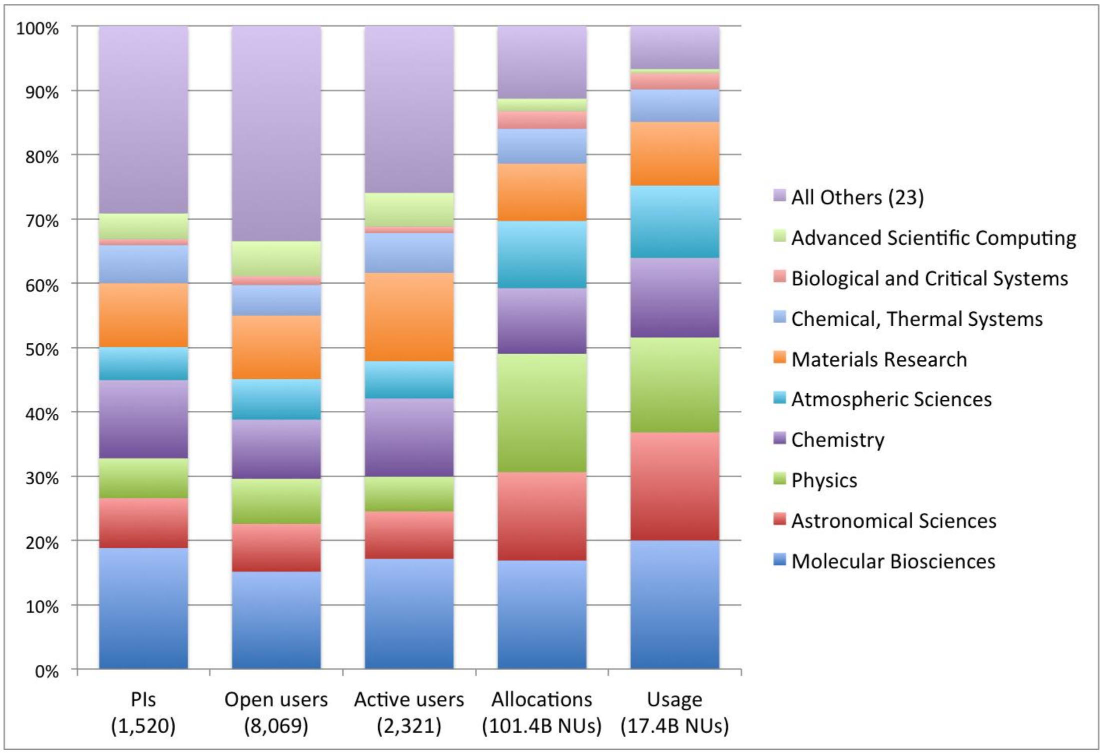


Figure 44. Quarterly XSEDE user, allocation, and usage summary by field of science, in order by usage, excluding staff projects. Note: PIs, users may appear under more than one field of science.

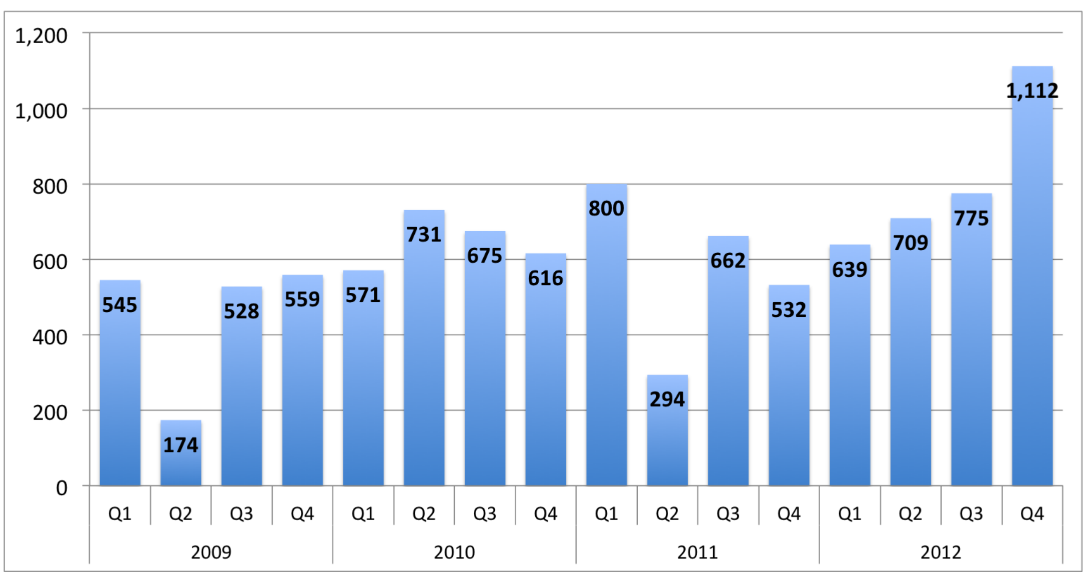


Figure 45. Publications, conference papers, and presentations reported by XSEDE users

Table 16. End of quarter XSEDE open user accounts by type, excluding XSEDE staff.

Category	Q1 2012	Q2 2012	Q3 2012	Q4 2012
Graduate Student	2,466	2,574	2,678	2,555
Faculty	1,293	1,344	1,386	1,322
Postdoctorate	1,059	1,075	1,109	1,002
Undergraduate Student	587	639	733	627
University Research Staff (excluding postdocs)	509	535	559	492
High school	5	4	10	13
Others	394	465	489	453
TOTALS	***6,313***	***6,636***	***6,964***	***6,464***

Table 17. Active institutions in selected categories. Institutions may be in more than one category.

Category		Q1 2012	Q2 2012	Q3 2012	Q4 2012
Campus Champions	Sites	59	62	69	65
	Users	776	795	812	876
	% total NUs	39%	45%	39%	34%
EPSCoR states	Sites	64	67	66	61
	Users	287	318	324	321
	% total NUs	16%	20%	15%	17%
MSIs	Sites	13	18	17	15
	Users	33	40	37	38
	% total NUs	1%	1%	1%	0.4%
International	Sites	52	63	44	36
	Users	83	86	70	61
	% total NUs	3%	3%	2%	4%

E.1.2 Project and allocation metrics

Figure 46 shows the five-year trend for requests and awards at XSEDE quarterly allocation meetings. The figure shows the continued strong growth in demand even with the 40% increase in available resources due to the first allocations on the TACC Stampede system. NUs requested were 229% of NUs available, and the XRAC recommendations were 122% of the NUs available. XSEDE awarded slightly fewer NUs than recommended because requests could not be moved to alternate resources in all cases, due to architectural differences. Table 18 presents a summary of overall project activity. Notably, 89% of XRAC requests received an award, and 38% were new awards.

Table 19 shows projects and activity in key project categories as reflected in allocation board type, including the number of open and active user accounts with each type of project. (Science Gateways may appear under any board.).

Table 20 shows detailed information about allocations activity for the various request types available for the different classes of projects. Notably, XSEDE had 188 Research (XRAC) requests, an all-time high; for the first time, XRAC requests exceeded the number of Startup, Education, and Campus Champion requests combined. Of the XRAC requests, 168 (89%) received awards, including 63 new projects. There were also 142 Startup requests, of which 109 (78%) received awards; 13 Education requests with 12 awards; and 23 Campus Champion requests with 22 awards.

As a special class of projects, science gateway activity is detailed in Figure 47, showing continued high levels of usage and users from these projects.

Table 21 shows gateway activity supported by specific XSEDE resources.

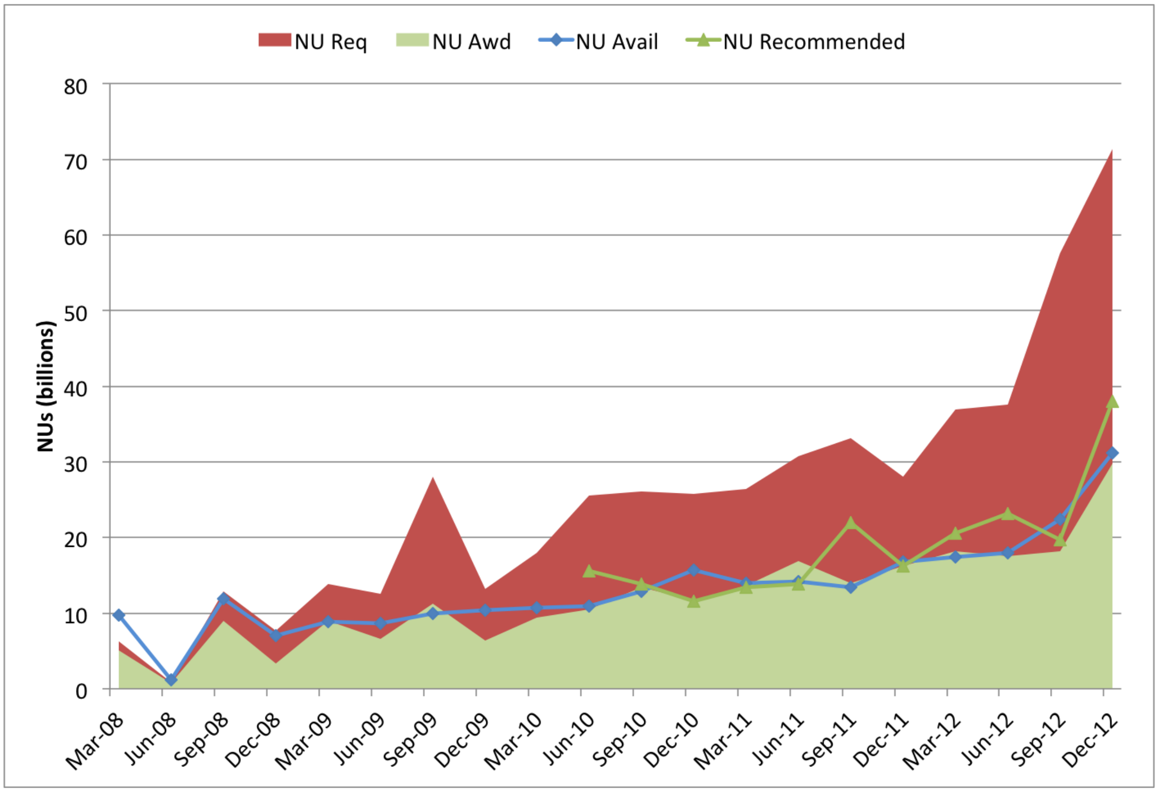


Figure 46. Allocation meeting history, showing NUs requested, awarded, available, and recommended. June 2008 was the last MRAC meeting with only "medium" requests.

Table 18. Project summary metrics

Project metric	Q1 2012	Q2 2012	Q3 2012	Q4 2012
XRAC requests	123	147	158	188
XRAC request success	96%	90%	87%	89%
XRAC new awards	36%	39%	36%	38%
Startup requests	168	206	176	142
Startup request success	89%	82%	81%	78%
Projects open	1,545	1,600	1,612	1,606
Projects new	216	247	212	201
Projects active	979	1,027	1,028	1,014
Projects closed	219	207	218	229
Resource diversity (wtd)	1.4 (1.9)	1.5 (2.0)	1.5 (2.1)	1.4 (2.0)
SP diversity (wtd)	1.3 (1.6)	1.3 (1.7)	1.3 (1.7)	1.3 (1.6)

Table 19. Project activity by allocation board type.

Board	Open projects	Open users	Active projects	Active users	NUs
XRAC	619	4,375	547	1,431	16,687,742,922
Startup	789	1,769	376	485	553,422,856
Campus Champions	100	608	35	69	71,979,222
Educational	71	1,378	44	425	56,517,041
Staff	27	526	15	121	7,280,760
Discretionary	0	0	2	6	186,150
Totals	1,606	8,656	1,019	2,537	17,377,128,951

Table 20. Allocations activity in POPS, excluding staff and discretionary projects.

	Research				Startup			
	# Req	SUs Req	# Awd	SUs Awd	# Req	SUs Req	# Awd	SUs Awd
New	73	227,633,708	64	85,902,706	130	21,152,223	101	11,749,047
Prog. Report	n/a				n/a			
Renewal	115	807,600,507	105	341,830,627	12	1,348,526	8	810,014
Advance	36	14,671,446	32	10,331,000	n/a			
Justification	8	15,595,500	1	3,100,000	0	0	0	0
Supplemental	28	34,547,494	8	4,071,000	11	2,280,015	9	905,000
Transfer	88	40,805,108	82	24,039,162	34	2,115,824	31	1,679,017
Extension	56	n/a	47	n/a	32	n/a	31	n/a
	Education				**Campus Champions**			
	# Req	SUs Req	# Awd	SUs Awd	# Req	SUs Req	# Awd	SUs Awd
New	6	630,210	5	480,000	8	7,478,047	7	4,449,005
Prog. Report	n/a				n/a			
Renewal	7	2,221,012	7	2,210,000	15	11,415,015	15	7,001,009
Advance	n/a				n/a			
Justification	0	0	0	0	0	0	0	0
Supplemental	5	264,000	5	254,000	9	605,000	6	425,000
Transfer	1	1,800	0	0	0	0	0	0
Extension	4	n/a	4	n/a	0	n/a	1	n/a

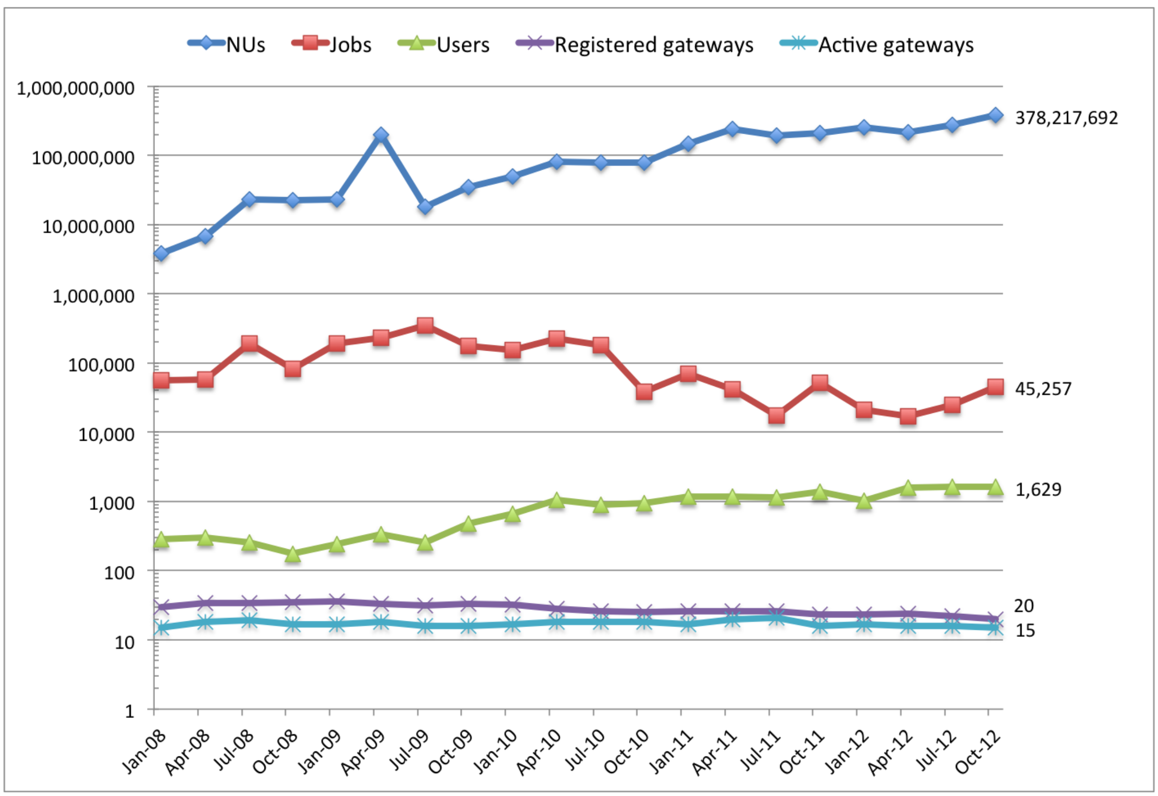


Figure 47. Quarterly gateway usage (NUs), jobs submitted, users (reported by ECSS), registered gateways, and active gateways.

Table 21. Gateway activity by resource.

Resource	Gateways	Jobs	NUs
SDSC Gordon	3	17,940	179,057,574
SDSC Trestles	6	19,723	99,097,599
NICS Kraken	4	5,078	59,253,226
TACC Ranger	9	987	26,945,205
TACC Lonestar	3	966	11,821,706
PSC Blacklight	1	166	1,999,436
Purdue Steele	3	397	42,946

E.1.3 Resource and usage metrics

In Q4, SP systems delivered 17.3 billion NUs, a decrease of about 4% from the previous quarter, but 13% more NUs than the year-ago quarter. Table 22 breaks out the resource activity according to different resource types. Figure 48 shows the total NUs delivered by XSEDE computing systems, as reported to the central accounting system over the past five years.

Figure 49 presents a perspective of the capacity and capability use of XSEDE resources by project. The figure shows the cumulative percentage of projects and resource usage according to each project's largest reported job size (in cores). The point at which the proverbial 80/20 rule holds precisely is at 74/26; that is the 74% of projects whose largest jobs were between 512 and 1,024 cores consumed only 26% of the delivered NUs, while the remaining 26% of projects, whose largest jobs were all of larger sizes, consumed the remaining 74% of delivered NUs.

Finally, Table 23 presents some summary metrics to reflect aggregate "usage satisfaction," including the average run time, wait time, response time (run + wait), and slow down (or expansion factor). These values are presented as unweighted averages, which show the impact of small jobs, and as averages weighted by each job's portion of the workload (in core-hours), which show responsiveness to the jobs responsible for most of the delivered NUs. Notably for Q4, while the "average" job is only 2 hours long, the average weighted job is just more than 23 hours long, and all the weighted usage satisfaction metrics showed decreases, an indicator of faster responsiveness and thus user satisfaction. The weighted average for slow down (3.6) eliminates the skew in the job slow down attributed to small jobs and shows a much more realistic average perceived slowdown for the work delivered.

XSEDE provides central monitoring of GRAM5 job submission activity at XSEDE SP sites (Figure 50). GRAM has been deprecated in favor of GRAM5, and thus we are no longer reporting pre-GRAM5 jobs separately.

Table 22. Resource activity, by type of resource, excluding staff projects.
Note: A user will be counted for each type of resource used.

Type	Resources	Jobs	Users	NUs
High-performance computing	6	1,234,540	1,824	15,233,456,536
Data-intensive computing	2	99,166	498	1,994,539,728
Visualization system	3	8,645	106	95,768,362
High-throughput computing	2	275,382	16	46,083,563
Totals	13	1,617,733	2,444	17,369,848,189

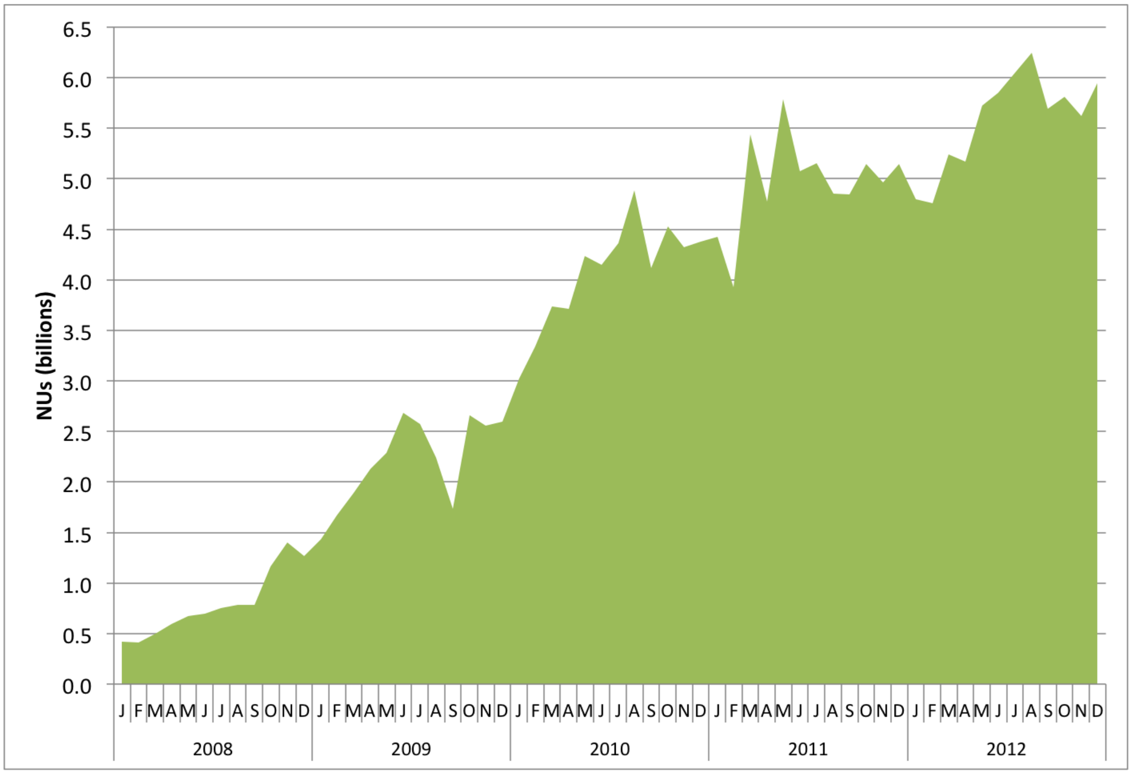


Figure 48. Total XSEDE resource usage in NUs.

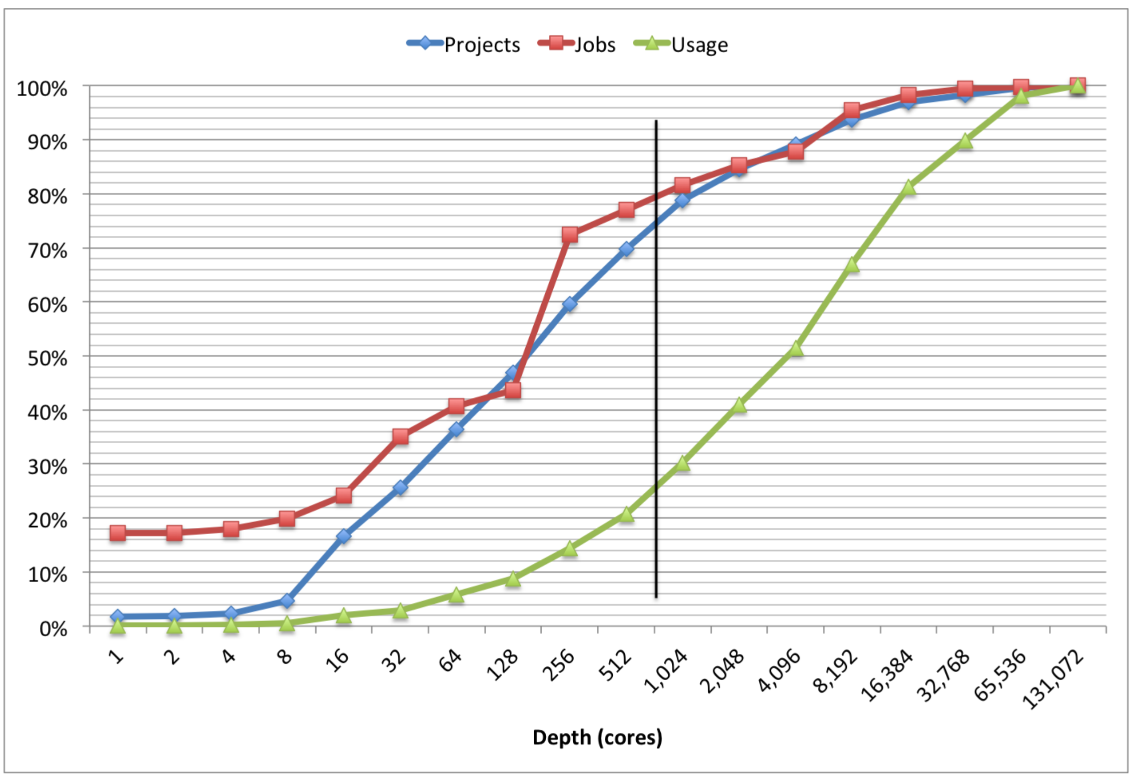


Figure 49. Cumulative distribution of projects, jobs, and usage according to project's maximum job size in cores (excludes staff projects). Vertical line (black) shows "joint ratio" of 74/26 at between 512 and 1,024 cores. I.e., 74% of projects use fewer than (a bit less than) 1,024 cores and consume 26% of XSEDE NUs; the other 26% of projects have larger jobs and consume the other 74% of XSEDE NUs.

Table 23. Usage satisfaction metrics, for HPC and data-intensive computing resources only, excluding staff projects.

	Job attribute	Q1 2012	Q2 2012	Q3 2012	Q4 2012
Unweighted average	Run time (hrs)	5.0	2.0	2.0	2.0
	Wait time (hrs)	6.1	4.4	6.2	4.4
	Response time (hrs)	12.1	7.3	9.7	7.6
	Slow down	334.4	324.7	512.2	334.0
Weighted average	Wtd run time (hrs)	23.3	20.9	22.4	23.4
	Wtd wait time (hrs)	23.2	32.6	36.5	30.1
	Wtd response time (hrs)	46.5	53.5	58.9	53.5
	Wtd slow down	3.3	4.7	4.1	3.6

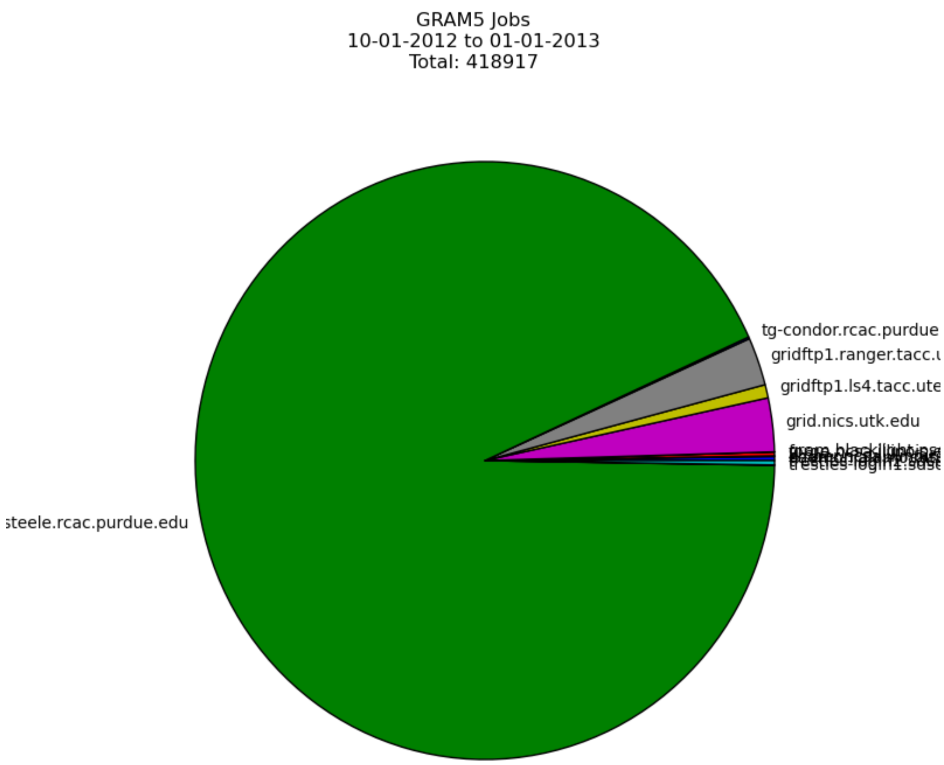


Figure 50. GRAM5 jobs by site 07-01-2012 to 10-01-2012

E.2 XSEDE Program Metrics

E.2.1 Project Office 1.1

1.1.4 External Relations

The XSEDE External Relations team reported the following media hits for the quarter.

Table 24. XSEDE media hits.

Date	Source	Headline	Notes
10/2/12	Globe Newswire	The Apache Software Foundation Announces Apache Rave as a Top-Level Project	
10/3/12	HPCwire	NSF-NCSA Study Probes Relationship between Industrial Applications and Underlying Science	
10/4/12	HPCwire	Researchers Study the Effects of Supercomputing on Wall Street	Good story to showcase importance of XSEDE resources

Date	Source	Headline	Notes
10/5/12	InsideHPC	Using Supercomputers to Regulate High-Frequency Trading	Wall Street
10/5/12	h-online.com	Apache Airavata becomes Top-Level Project	
10/5/12	eWeek.com	Apache Airavata Graduates to Top-Level Project	
10/8/12	HPCwire	I-CHASS awarded $99,986 from National Science Foundation	
10/11/12	HPCwire	San Diego Supercomputing Center to Host Data for Metabolomics Study	
10/16/12	HPCwire	Cornell Offers Parallel Computing Training for 'Stampede' Supercomputer	
10/17/12	ISGTW	Keeping an eye on superfast transactions on Wall Street	We pitched this
10/23/12	HPC In the Cloud	Promoting Hemispheric Advancement Through Collaborative Research	I-CHASS
10/25/12	UW News	UW Faculty Members Have Dec. 17 to Submit Large Allocation Requests to Use Supercomputer in 2013	links to XSEDE homepage
10/31/12	Sys-con Media	Conquering Data-Intensive BioScience Problems: An SGI Webinar	Blog feed post
11/1/11	Compute Calcul Canada	Compute Canada Calcul Canada Inaugural Board of Directors Will Advance Canada's Research and Innovation Agenda	
11/2/12	Science Codex	Cancer bound	Same as medicalxpress.com
11/2/12	Medicalxpress.com	Researchers use supercomputer simulations to understand how some carcinogens evade removal	Same as Science Codex
11/2/12	HPCwire	XSEDE13 Calls for Participation	
11/7/12	EurekAlert!	A firm molecular handshake needed for hearing and balance	PSC
11/7/12	HPCwire	Computer Simulations Shed Light on Cancer Prevention	TACC
11/7/12	HPCwire	PSC's Sherlock to Solve Big Data Mysteries	featured in XSEDE external newsletter
11/12/12	equities.com	HP ProLiant Servers Deliver Extreme Compute Performance	Keeneland, story out of SC12
11/13/12	KUTV	The World's Smartest Computers are in Salt Lake	Presence at SC12
11/14/12	HPCwire	Keeneland Project Deploys GPU Super for NSF	
11/27/12	EurekAlert!	Upgrade to visualization and analysis system eases path for beginning supercomputer users	RDAV
11/27/12	Tribuna Economica	Iserver HP ProLiant Offrono Prestazini Di Calcolo Eccezionali	Keeneland
11/27/12	HPCwire	Lifka Elected National Chair of CASC	
11/27/12	HPCwire	Tapia Conference Registration Opens	
11/28/12	Indiana University	IU selected as home for US Desk of international scientific computing publication: University Information Technology Services News Room: Indiana University	
11/30/12	HPCwire	CMU, PSC Awarded $9.3 Million for Bio Systems Modeling	PSC
12/5/12	Science360 News Service (NSF)	The Dark Energy Survey	DES

E.2.2 Operations 1.2

1.2.1 Security

The XSEDE security team has identified the following metrics for tracking security incidents and response. summarizes the metrics, and details on any incidents are provided in the main body of the report. Of the two compromised accounts, one was reactivated after a password change, while the other user never responded to emails/calls from staff and remains suspended.

Table 25. XSEDE security metrics and incident response

	Q1 2012	Q2 2012	Q3 2012	Q4 2012
XSEDE-wide notice of vulnerability	0	0	0	0
Compromised user accounts	0	0	2	0
Other incident response	0	0	0	0
Critical rollout of vulnerability patches	0	0	0	0
Security enhancement rollouts	0	1	0	1

1.2.2 Data Services

XSEDE supports monitoring for two central data movement services: the gridFTP service connecting the XSEDE service providers and the Globus Online service for connecting XSEDE service providers as well as external sites. Table 26 shows quarterly summary metrics and increasing Globus Online adoption over the past four quarters, while Figure 51 and Figure 52show Globus Online and GridFTP activity, respectively, by SP site.

Table 26. Globus Online activity to and from XSEDE endpoints, excluding GO XSEDE speed page user.

		Q1 2012	Q2 2012	Q3 2012	Q4 2012
To/from XSEDE endpoint	Files to XSEDE	27.6 million	34.8 million	57.1 million	14.1 million
	TB to XSEDE	232	824	311	559
	Files from XSEDE	17.8 million	23.9 million	44.9 million	17.7 million
	TB from XSEDE	242	185	325	453
	Faults detected	584,000	971,000	985,000	1,561,000
	Users	149	187	218	217
To/from XSEDE via Globus Connect	Files to XSEDE	6.3 million	2.5 million	24.9 million	2.1 million
	TB to XSEDE	45	18	37	37
	Files from XSEDE	0.6 million	2.2 million	9.4 million	4.9 million
	TB from XSEDE	25	11	34	23
	Faults detected	242,000	381,000	575,000	770,000
	Users	87	97	138	124

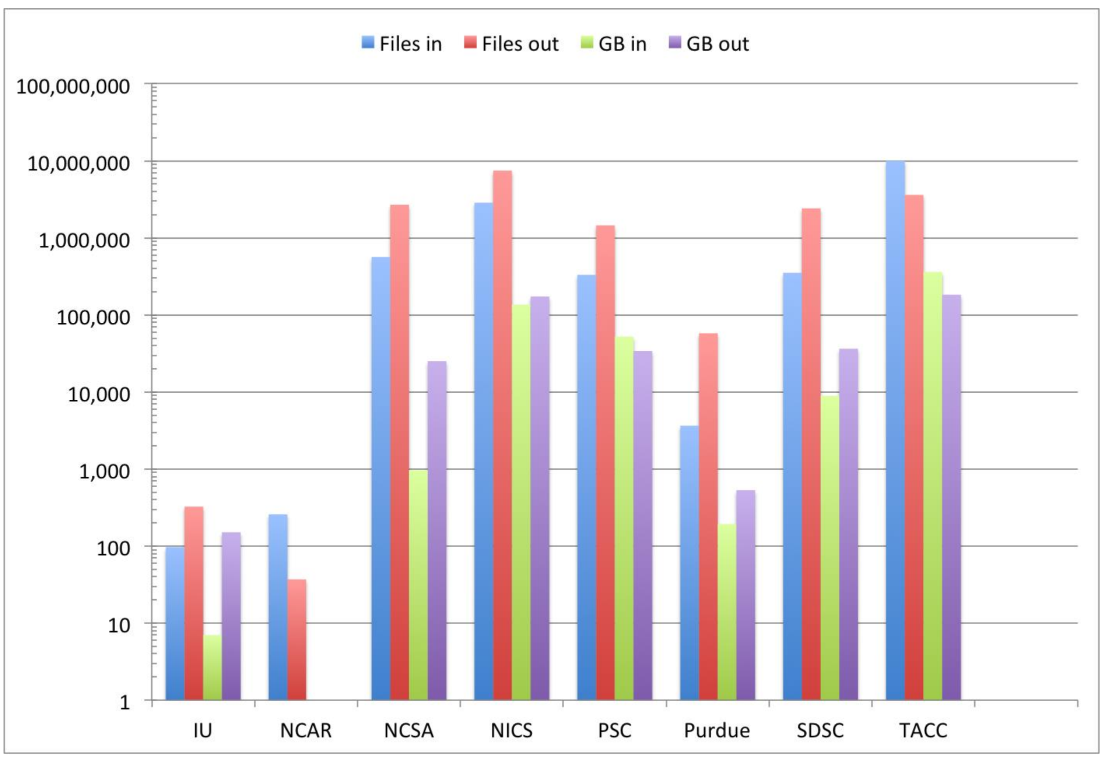


Figure 51. Globus Online activity into and out of XSEDE SP end points

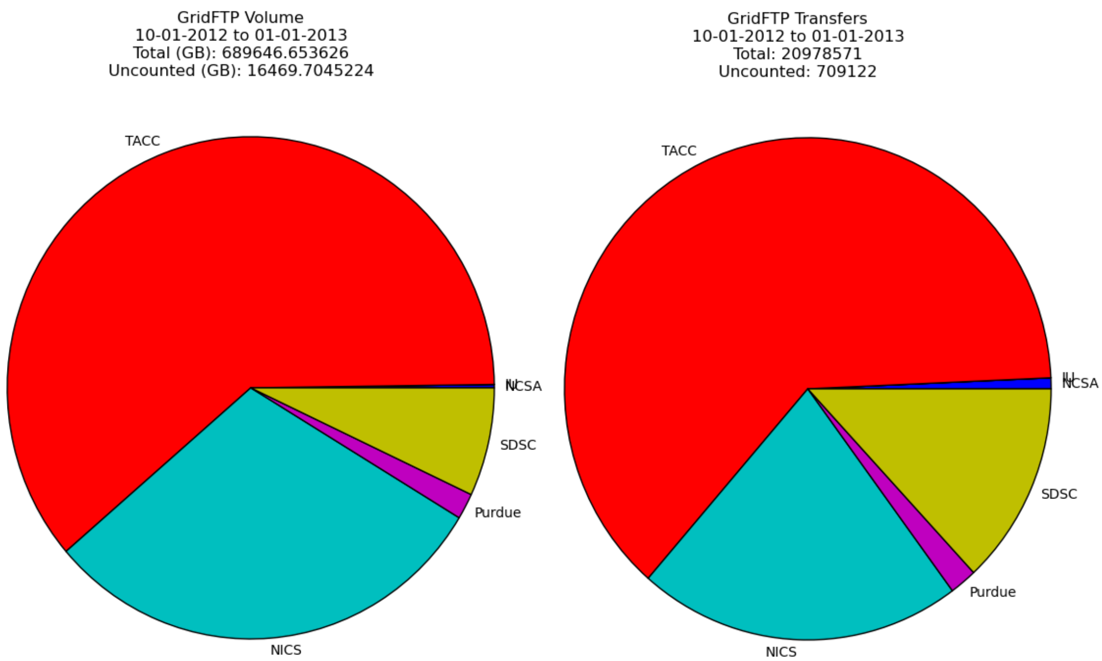


Figure 52. GridFTP volume and file transfers, per SP site.

1.2.3 XSEDEnet

Traffic utilization of the Chicago-Denver XSEDEnet link is shown in two figures below. Figure 53 shows the peak bandwidth across the link for the period. Figure 54 shows link utilization as a percentage. Traffic across all XSEDEnet links is shown in Figure 55.

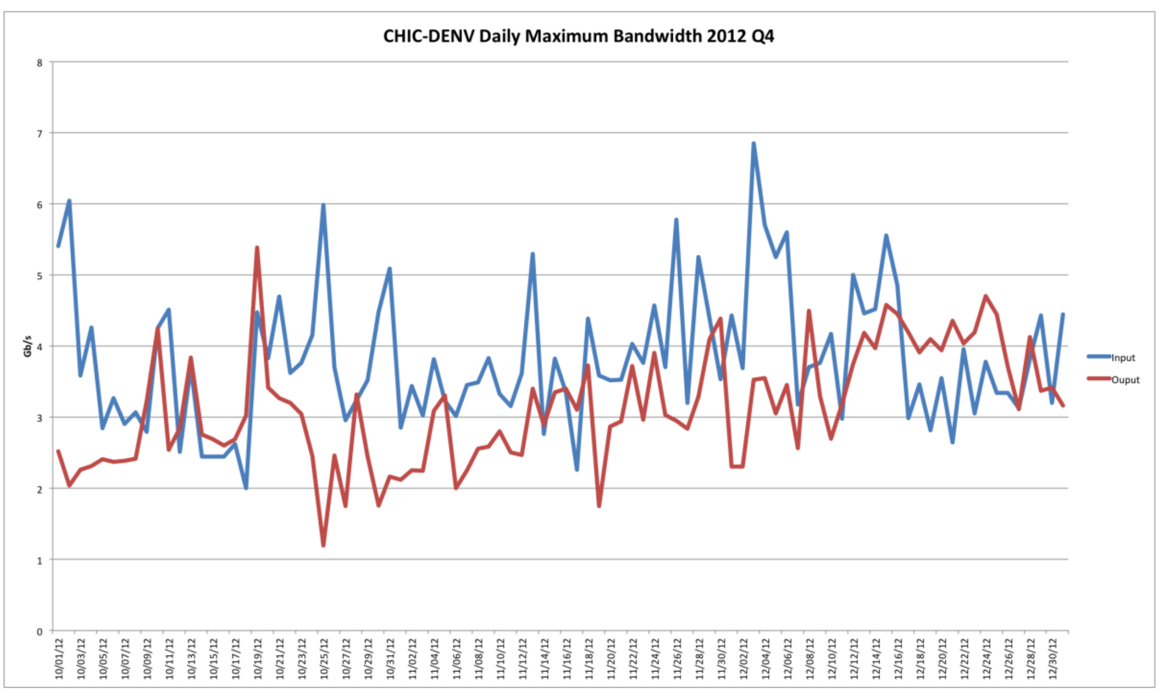


Figure 53. XSEDEnet Chicago-Denver peak bandwidth

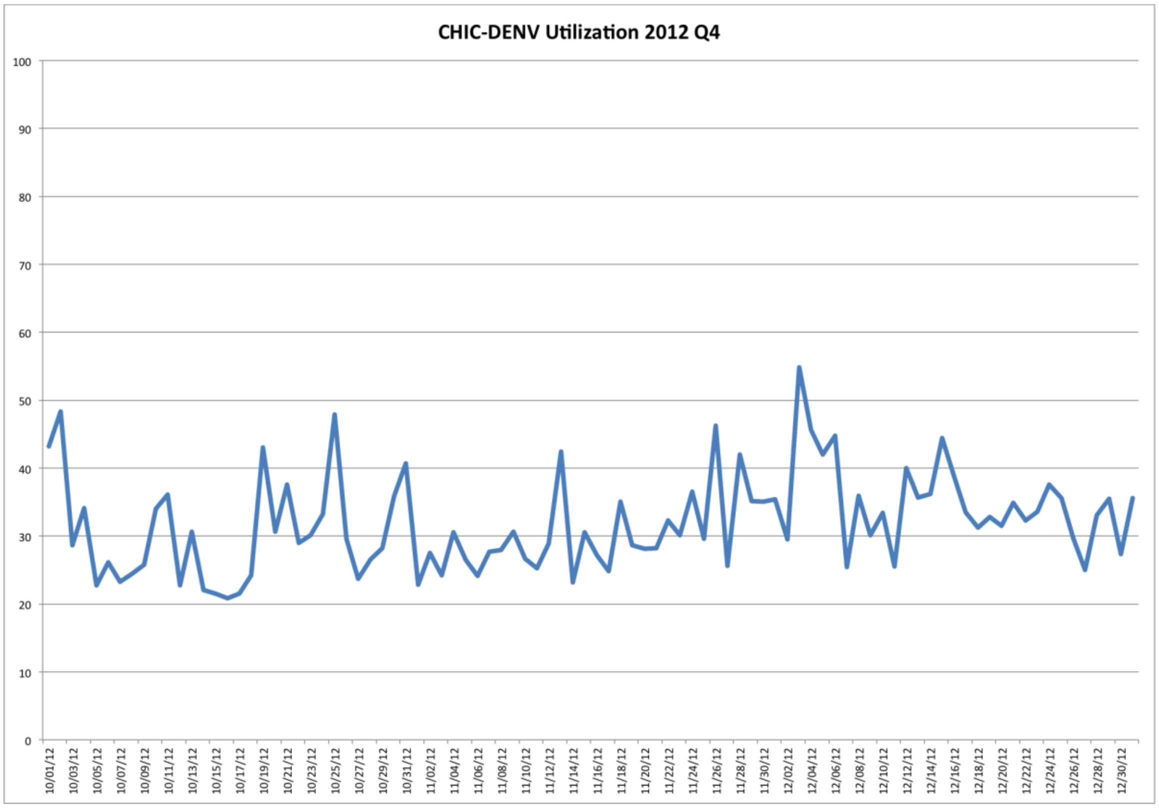


Figure 54. XSEDEnet Chicago-Denver utilization (as a percentage)

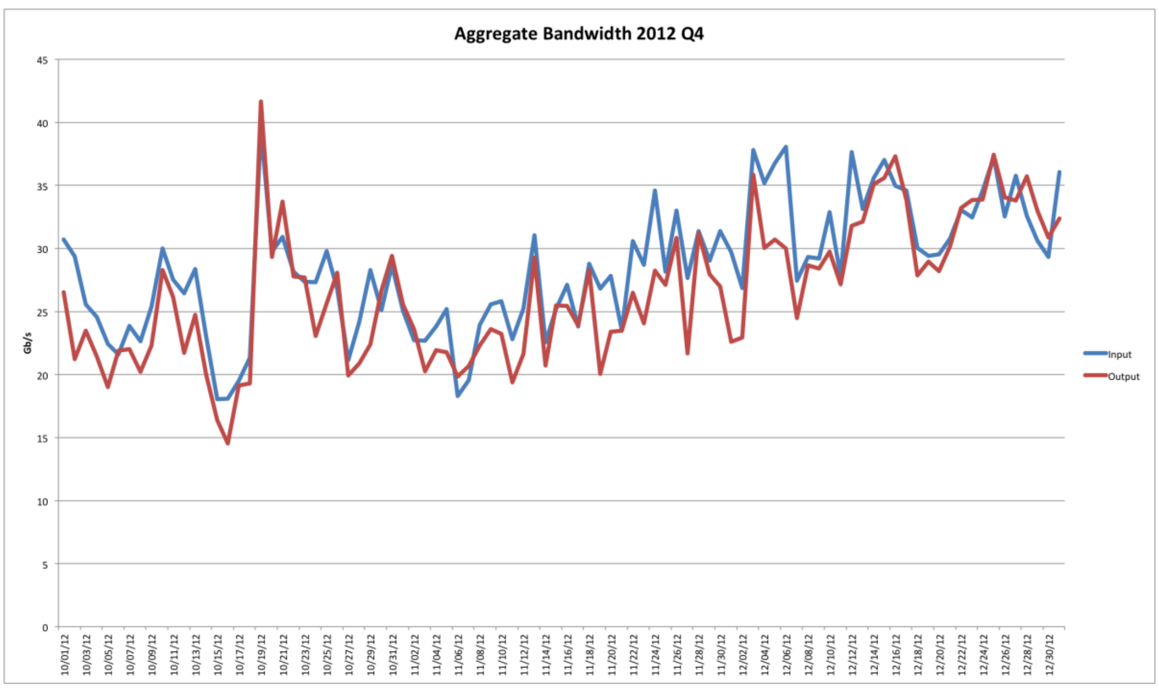


Figure 55. XSEDEnet Q3 2012 aggregate bandwidth across all links

1.2.5 Accounting and Account Management

The Accounting and Account Management group administers and operates the software for the XSEDE allocations system (POPS), the accounting system, and user account management. Table 27 shows the processing time for ongoing allocation requests outside of the quarterly XRAC requests. XSEDE reduced the account creation time to a matter of minutes with the deployment of POPS and User Portal components that allow users to create their own portal logins.

Table 27. Average time to process allocation requests and account creation requests, in days. (Excludes quarterly XRAC requests; "n/a" indicates none submitted.)

ALLOCATION REQUESTS		Q1 2012	Q2 2012	Q3 2012	Q4 2012
Research	Advance	6	7	5	12
	Transfer	3	3	5	3
	Supplement	25	14	7	17
	Justification	15	n/a	44	5
Startup, Education, Campus Champions, Discretionary	New	9	9	10	12
	Renewal	10	6	3	7
	Transfer	3	3	4	3
	Supplement	4	4	8	5
Account creation requests		1.8	0.03	0.03	0.03

1.2.6 Systems Operational Support

The Systems Operational Support group encompasses the XSEDE Operations Center (XOC), which includes front-line user support and the ticket system, and the system administration of all XSEDE centralized services. In the ticket system, XSEDE tracks total ticket volume and responsiveness (Table 28), which groups ("resolution centers") field the tickets (Table 29), and the numbers of tickets in seven common categories (Table 30 and Figure 56). The totals by resolution center and by category do not add up to the total number of tickets opened and closed because some tickets are resolved by staff not in a resolution center and some resolution centers have non-standard categories.

For the central services, XSEDE tracks the uptime reported by system administrators (

Table 31) as well as the Inca-reported uptime for seven key user-visible services (Table 32). The Inca-reported uptime better reflects "user-visible outages," that is, what the average user would experience, and typically exceeds the actual system uptime, reflecting the effectiveness of XSEDE's backup systems, failover capabilities, and operational responsiveness.

Table 28. XSEDE Operations Center ticket system metrics.

	Q1 2012	**Q2 2012**	**Q3 2012**	**Q4 2012**
Total tickets opened	2,651	2,744	2,421	2,098
Tickets opened – email	2,381	2,448	2,175	1,872
Tickets opened – portal	254	26	18	18
Tickets opened – phone	16	270	228	208
Total tickets closed	2,335	2,394	2,028	2,021
Tickets, response in 24 hrs	2,263 (85%)	2,326 (85%)	2,021 (83%)	1,727 (82%)
Tickets closed within 2 bus. days	1,044 (39%)	1,050 (38%)	880 (36%)	742 (35%)

Table 29. Ticket breakdown (opened/closed) for each major resolution center.

	Q1 2012		**Q2 2012**		**Q3 2012**		**Q4 2012**	
	Opened	**Closed**	**Open**	**Closed**	**Open**	**Closed**	**Open**	**Closed**
NICS	670	605	657	640	481	458	514	503
XOC	427	305	415	298	349	231	290	171
TACC	330	295	276	251	292	257	253	218
Proposal issues	343	251	408	376	403	358	381	300
SDSC	218	182	379	327	313	251	298	242
PSC	115	108	89	87	75	64	50	48
Purdue	69	58	118	115	82	82	60	60
NCSA	60	42	89	72	83	81	21	18
User facing services	88	68	73	65	25	22	67	65
UST	12	9	11	11	11	11	5	5
IU	7	1	10	7	3	3	2	2
OSG	2	1	3	3	1	1	2	1
Others	*335*	*258*	*215*	*135*	*303*	*209*	*153*	*85*

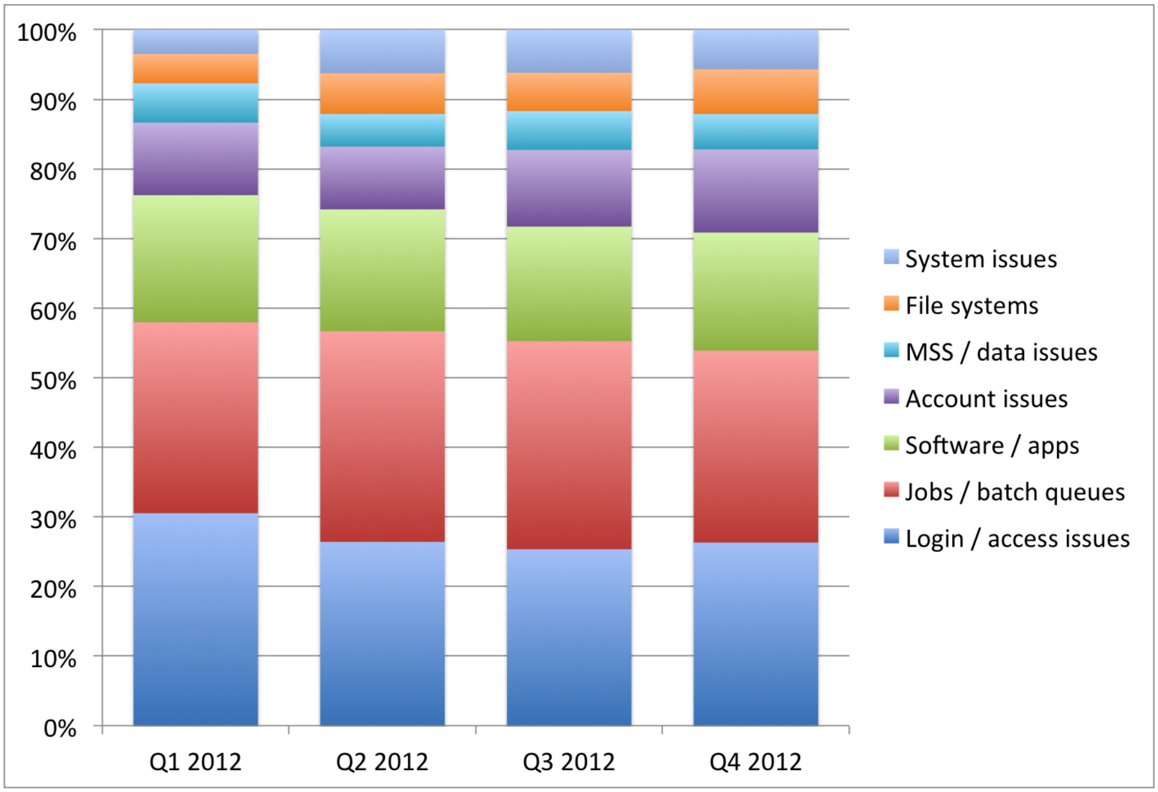


Figure 56. Tickets in seven primary problem categories. This chart represents a significant portion of tickets but does not represent the entire range. Tickets largely fit in the seven displayed categories; other categories are not significant enough to visually represent.

Table 30. Ticket counts for the seven primary problem categories shown in Figure 56.

	Q1 2012	Q2 2012	Q3 2012	Q4 2012
Login / access issues	483	445	345	326
Jobs / batch queues	434	510	407	342
Software / apps	289	295	224	210
Account issues	165	152	150	148
MSS / data issues	89	79	76	63
File systems	67	99	75	80
System issues	55	105	84	70

Table 31. XSEDE centralized service uptime and outages. Empty cells indicate *no outages (100% up)*. “% Up” is percent uptime; “Hrs (P|U)” shows outage hours, planned and unplanned.

Service	Q1 2012		Q2 2012		Q3 2012		Q4 2012	
	% Up	Hrs (P|U)	% Up	Hrs (P|U)	% Up	Hrs (P|U)	% Up	Hrs (P|U)
AMIE			99.91%	0|2				
AMIE backup	99.98%	0.5|0						
Bugzilla	97.46%	0|56	99.82%	4|0				
Build and Test	97.46%	0|56	99.82%	4|0				
Certificate Authority	99.62%	8.5|0					99.73%	0|6
Data Movement Service								
Globus Listener	97.46%	0|56	99.82%	4|0				
IIS Metrics	97.46%	0|56	99.82%	4|0				
Inca			99.31%	0|15	98.71%	26|2.5		
Inca backup			99.50%	11|0			99.91%	0|2
Information Services	97.46%	0|56	99.82%	4|0				
Karnak	97.40%	0|57.5	99.82%	4|0	99.98%	0|0.5	91.17%	0|195
Kerberos backup	99.91%	2|0.08						
Knowledgebase								
MyProxy								
Openfire Jabber								
POPS								
RDR	98.69%	5|24					99.64%	0|8
Sciforma					99.84%	3.5|0		
Secure Wiki								
SELS								
Sharepoint								
Software Distribution	97.46%	0|56	99.82%	4|0				
Source Repository	97.46%	0|56	99.82%	4|0				
Speedpage	99.91%	2|0			99.95%	1|0		
TG Wiki	97.46%	0|56	99.82%	4|0				
Ticket System								
Usage Reporting Tools								
User Portal	99.97%	0|0.75						
User Portal backup	99.62%	8.5|0	99.95%	1|0			99.91%	0|2
User Profile Service	97.46%	0|56						
XDCDB			99.91%	0|2	99.97%	0|0.75	99.90%	0.06|2.25
XDCDB backup	99.98%	0.5|0	99.91%	2|0	98.91%	0|24	99.64%	0|8

Table 32. Inca-monitored XSEDE central services, Inca-detected uptimes, and outages.

Service	Outage definition. Test frequency.	Q1 2012	Q2 2012	Q3 2012	Q4 2012
Inca	Inca status pages unavailable or test details page fails to load. Every 5 min.	100%	99.3%	98.71%	99.71%
Information Services	Information web pages unavailable. Every 15 min.	99.97%	99.9%	100%	99.76%
Karnak	Karnak front page fails to load. Every 30 min.	99.93%	99.9%	99.98%	91.17%
MyProxy	MyProxy server does not respond to credential check. Every hour.	100%	100%	100%	100%
User Portal	Portal home page fails to load correctly. Every 30 min.	99.98%	100%	99.98%	100%
XDCDB	Connection to database refused or slow (using check_postgres.pl script). Every 5 min.	100%	99.99%	99.96%	100%

E.2.3 User Services 1.3

1.3.1 Training

With the Q4 2012 report, we are including aggregate training metrics, including number of events held and attendees as well as online modules and visitors, in Table 33.

Table 33. Training events and attendees

	Q4 2012
Events held	23
Event attendees	858
Online modules available	41
Online module unique visitors	7,774
Online module repeat visitors	1,444

1.3.2 User Information & Interfaces

The User Information and Interfaces group provides XSEDE users with central information and services via the XSEDE User Portal (XUP), web site, XUP mobile, and knowledgebase. Table 34 shows increasing activity on most user information interfaces, as well as increases in the numbers of logged-in users accessing these interfaces. Table 35 shows the most popular XUP applications, by visits.

Table 34. XSEDE web site, user portal and XUP Mobile activity. (Note: "Users" indicates logged-in users.)

UII Activity	Q1 2012	Q2 2012	Q3 2012	Q4 2012
Web hits	2,667,120	2,676,532	2,362,105	2,269,506
Web visitors	38,502	33,362	33,053	33,145
XUP hits	1,340,704	1,465,537	1,540,402	1,558,209
XUP visitors	14,913	13,787	16,118	16,998
XUP accounts	6,159	7,563	9,015	10,000
XUP users	3,919	3,976	4,399	4,346
XUP users running jobs	1,554	1,552	1,552	1,640
XUP Mobile hits	1,307	1,693	1,931	3,569
XUP Mobile users	37	25	20	17
KB docs retrieved	68,619	57,451	87,987	187,966
Total KB docs	478	497	538	573
New KB docs	73	19	62	36

Table 35. XUP and Web site application visits. "Users" indicates logged-in users.

	Q4 2011		Q1 2012		Q2 2012		Q3 2012		Q4 2012	
Application	**Visits**	**Users**	**Visits**	**Users**	**Visits**	**Users**	**Visits**	**Users**	**Visits**	**Users**
Allocations/Usage	69,290	2,991	49,261	3,803	50,998	3,724	45,899	3,773	44,572	3,649
File Manager	60,009 (xfers)	60 (3.9 TB)	31,952 (xfers)	79 (2.5 TB)	21,375 (xfers)	78 (20 TB)	42,219 (xfrs)	97 (3.6 TB)	37,852	69 (10.3 TB)
User News	4,312	25	62,784	526	47,194	2,013	25,707	263	26,992	338
GSI-SSH	34,132	1,083	24,714	1,343	28,317	1,354	22,411	1,286	21,352	1,248
Training Regis'n	12,648	345	19,535	828	11,642	631	10,556	650	18,726	1,011
Resource Listing	100,544	864	36,244	1,104	22,483	1,265	16,934	1,391	16,869	1,436
Publications							2,908	595	12,528	1,372
RSS news feed ***(tracking as of Q4)***									11,959	92
Help Desk/Consult	6,206	557	4,659	748	4,815	733	4,704	652	10,031	721
Software Search	14,812	176	8,204	265	8,879	316	9,903	318	9,707	344
System Accounts	13,457	1,609	12,897	1,841	12,235	1,813	10,919	1,731	9,037	1,632
Knowledge Base	17,454	261	11,436	377	10,964	338	8,269	156	8,699	217
System Monitor	13,350	1,050	8,213	1,257	9,401	1,034	6,819	985	6,996	888
User Profile			1,954	833	5,476	1,262	5,930	1,345	6,314	1,312
POPS Submit					5,639	1,204	5,982	1,117	5,735	1,118

	Q4 2011		Q1 2012		Q2 2012		Q3 2012		Q4 2012	
Application	**Visits**	**Users**	**Visits**	**Users**	**Visits**	**Users**	**Visits**	**Users**	**Visits**	**Users**
Gateways List	51,684	180	16,338	229	8,914	234	5,470	158	5,043	152
Add User Form	8,406	611	5,751	626	4,628	617	4,446	547	3,710	523
My Jobs	5,640	908	3,500	960	3,195	900	2,634	788	2,484	777
Ticketing System	3,708	609	2,366	682	2,600	654	2,229	609	1,996	532
Online Training Listing	2,720	215	2,093	347	1,668	437	1,414	220	1,452	304
SU Calculator	4,376	180	2,048	243	1,466	239	1,240	109	1,336	188
Karnak Q Predict	1,770	212	1,108	222	871	264	643	182	601	153
XSEDE Tech DB (***new in Q4 2012***)									330	15
Feedback form	1,174	57	791	53	426	39	333	17	319	11
Community Accts					436	311	318	259	279	206
Gateway Regis'n					243	16	238	8	275	12
DN Listing	1,092	399	554	371	450	326	127	99	*Now in User profile*	

E.2.4 Extended Collaborative Support Service 1.4, 1.5

The Extended Collaborative Support Service pairs members of the XSEDE user community with expert staff in projects lasting up to a year to solve challenging science and engineering problems. Table 36 shows project and staffing metrics. Table 37 shows metrics for Extended Support for Training, Education, and Outreach.

Table 36. Extended Collaborative Support project and staffing activity

		Q1 2012	**Q2 2012**	**Q3 2012**	**Q4 2012**
Project requests	XRAC	22	20	14	14
	Supplemental/Startups	41	28	30	18
	ECSS In-house project	1	0	0	0
Projects initiated	Research Team	19	14	15	13
	Community Codes	8	7	3	7
	Science Gateways	6	6	2	1
	Unassigned	7	0	2	1
Projects cancelled/no-go	XRAC	4	5	5	0
	Supplemental/Startups	20	16	17	10
Projects active	Research Team (XRAC)	27	29	26	30
	Research Team (S/S)	17	20	19	24
	Research (TG)	12	1	0	0
	Subtotal	**56**	**50**	**45**	**54**
	Community Codes (XRAC)	6	10	9	9
	Community Codes (S/S)	9	17	18	7
	Community Codes (TG)	2	2	1	0
	In-house	1	1	1	0
	Subtotal	**18**	**30**	**29**	**16**
	Science Gateways (XRAC)	4	9	9	7
	Science Gateways (S/S)	7	10	8	8
	Science Gateways (TG)	4	1	0	0
	Subtotal	**15**	**20**	**17**	**15**
	Total Projects Active	**89**	**100**	**91**	**85**
Work plans		14	10	14	9
Projects completed		16	15	11	11
Novel, Innovative Projects (NIP)	User groups engaged	20	47	65	72
	NIP-led ECS planning efforts	9	9	3	5
	NIP ECS requests (prospective user groups)	23	38	42	54
	NIP ECS projects active	7	9	10	10
	NIP outreach events	9	16	21	30

		Q1 2012	Q2 2012	Q3 2012	Q4 2012
ECSS staffing (FTE)	Research Team	13.28	12.8	13.19	15.54
	Community Codes	7.11	8.24	8.14	5.60
	Science Gateways	4.92	4.73	4.63	4.89
	NIP	5.79	5.64	5.64	5.05
	TEO	4.42	3.53	3.43	3.87
	Total	**35.52**	**34.94**	**35.03**	**34.95**

Table 37. Extended Support for Training, Education and Outreach 1.5.3

	Q1 2012		Q2 2012		Q3 2012		Q4 2012	
Description	**#**	**Staff**	**#**	**Staff**	**#**	**Staff**	**#**	**Staff**
Requests for service	4	4	2	2	0	0	4	4
User meetings and BOFs	2	2	18	20	11	12	13	13
Mentoring	3	2	12	12	9	9	2	2
Talks and presentations	12	9	20	20	15	22	9	12
Tutorials	21	25	31	32	12	18	5	10
Online tutorials and webinars	4	6	0	0	3	3	0	0
Online tutorial reviews	6	6	17	17	2	2	4	5

F XSEDE Publications Listing

F.1 XSEDE Staff Publications

F.1.1 Project Office 1.1

1. Stewart, C. A., "Campus Bridging Use Case - Initial Prioritization", Extreme Science and Discovery Environment (XSEDE) non-peer reviewed technical report, 2012. http://hdl.handle.net/2022/15214

F.1.2 Operations 1.2

F.1.3 User Services 1.3

2. Betro, V., Duque, E., Wyman, N. "Meshing, Visualization, and Computational Environments Technical Committee Year In Review." Aerospace America. Reston, VA. December 2012, p. 22.

F.1.4 Extended Collaborative Support – Projects 1.4, Communities 1.5

3. Harrison C., Navrátil P., Moussalem M., Jiang M., Childs H. "Efficient Dynamic Derived Field Generation on Many-Core Architectures Using Python" Proceedings of Workshop on Python for High Performance and Scientific Computing (PyHPC) 2012. November 16, 2012
4. Navrátil P., Barth W., Childs H. "Virtual Rheoscopic Fluids for Dense Large-Scale Fluid Flow Visualizations" Proceedings of IEEE Symposium on Large Data Analysis and Visualization (LDAV) 2012. October 14-15, 2012
5. Johnson J., Abram G., Westing B., Navratil P., Gaither K. "DisplayCluster: An Interactive Visualization Environment for Tiled Displays" Proceedings of IEEE Cluster 2012
6. Arora R., Bangalore P., Mernik M. "Techniques for Non-invasive Explicit Parallelization" Journal of Supercomputing, 62/3/1583-1608
7. Kuhn V., Craig A., Arora R., Bock D., Cai D., Franklin K., Marini L., Simeone M. "Large Scale Video Analytics: On-demand, Iterative Inquiry for Moving Image Research" eScience 2012
8. Kuhn V., Craig A., Arora R. "Multiple Concurrent Queries on Demand: Large Scale Video Analysis in a Flash Memory Environment as a Case for Humanities Supercomputing" XSEDE '12 Proceedings of the 1st Conference of the Extreme Science and Engineeering Discovery Environment: Bridging from the eXtreme to the Campus and Beyond
9. James D. "Having it Both Ways: Eclipse PTP on Desktop and Cluster" Presentation at Scientific Software Days 2012, Austin, TX

F.1.5 Education and Outreach 1.6

F.2 Publications from XSEDE Users

The following publications were gathered from Research submissions to the December 2012 XSEDE Resource Allocations Committee (XRAC) meeting. Renewal submissions are required to provide a file specifically to identify publications resulting from the work conducted in the prior year. The publications are organized by the proposal with which they were associated. This quarter, 122 requests identified 1,112 publications and conference papers that were published, in press, accepted, submitted, or in preparation.

1. ASC050025

1. Abhishek Gupta, Gengbin Zheng, and Laxmikant V. Kale. A multi-level scalable startup for parallel applications. In Proceedings of International Workshop on Runtime and Operating Systems for Supercomputers, Tucson, AZ, USA, 5 2011.
2. Akhil Langer, Ramprasad Venkataraman, Udatta Palekar, Laxmikant V. Kale, and Steven Baker. Performance Optimization of a Parallel, Two Stage Stochastic Linear Program: The Military Aircraft Allocation Problem. In Proceedings of the 18th International Conference on Parallel and Distributed Systems (ICPADS 2012). To Appear, Singapore, December 2012.
3. Jonathan Lifflander, Phil Miller, Ramprasad Venkataraman, Anshu Arya, Terry Jones, and Laxmikant Kale. Mapping dense lu factorization on multicore supercomputer nodes. In Proceedings of IEEE International Parallel and Distributed Processing Symposium 2012, May 2012.

4. Esteban Meneses, Greg Bronevetsky, and Laxmikant V. Kale. Dynamic load balance for optimized message logging in fault tolerant hpc applications. In IEEE International Conference on Cluster Computing (Cluster) 2011, September 2011.
5. Esteban Meneses, Xiang Ni, and L. V. Kale. A Message-Logging Protocol for Multicore Systems. In Proceedings of the 2nd Workshop on Fault-Tolerance for HPC at Extreme Scale (FTXS), Boston, USA, June 2012.
6. Esteban Meneses, Osman Sarood, and L. V. Kale. Assessing Energy Efficiency of Fault Tolerance Protocols for HPC Systems. In Proceedings of the 2012 IEEE 24th International Symposium on Computer Architecture and High Performance Computing (SBAC-PAD 2012), New York, USA, October 2012.
7. Harshitha Menon, Nikhil Jain, Gengbin Zheng, and Laxmikant V. Kal´e. Automated load balancing invocation based on application characteristics. In IEEE Cluster 12, Beijing, China, September 2012.
8. Phil Miller, Shen Li, and Chao Mei. Asynchronous collective output with non-dedicated cores. In Workshop on Interfaces and Architectures for Scientific Data Storage, September 2011.
9. Xiang Ni. A semi-blocking checkpoint protocol to minimize checkpoint overhead. Master's thesis, Dept. of Computer Science, University of Illinois, 2012. http://charm.cs.uiuc.edu/newPapers/12-15.
10. Xiang Ni, Esteban Meneses, and Laxmikant V. Kal´e. Hiding checkpoint overhead in hpc applications with a semi-blocking algorithm. In IEEE Cluster 12, Beijing, China, September 2012.
11. Gengbin Zheng, Stas Negara, Celso L. Mendes, Eduardo R. Rodrigues, and Laxmikant V. Kale. Automatic handling of global variables for multi-threaded mpi programs. In Proceedings of the 16th International Conference on Parallel and Distributed Systems (ICPADS) 2011, number 11-23, December 2011.

2. ASC090004

12. Jun Wu and Francois Gygi, A simplified implementation of van der Waals density functionals for first-principles molecular dynamics applications. The Journal of chemical physics, 2012. **136**(22): p. 224107.
13. Gary Yuan and Francois Gygi, A distributed approach to verification and validation of electronic structure simulation data using ESTEST. Computer physics communications, 2012. **183**(8): p. 1744-1748.
14. F. Gygi and I. Duchemin, Efficient Computation of Hartree-Fock Exchange using Recursive Subspace Bisection, submitted to JCTC (8/10/2012).

3. ASC100002

15. P. S. Rawat and X. Zhong, "Direct Numerical Simulations of Turbulent Flow Interactions with Strong Shocks Using Shock-Fitting Method," under review for Journal of Fluid Mechanics, 2012.
16. X. Wang and X. Zhong, "The stabilization of a hypersonic boundary layer using local sections of porous coating," Physics of Fluids, Vol. 24, 034105 (1-28), 2012.
17. X. Zhong and X. Wang, "Direct numerical simulation on the receptivity, instability, and transition of hypersonic boundary layers," Annual Review of Fluid Mechanics, Vol. 44, pp. 527-561, 2012.
18. X. Wang, and X. Zhong, "Strong shock and turbulence interactions w/ or w/o thermochemical non-equilibrium effects," 65th Annual Meeting of the APS Division of Fluid Dynamics, 2012.
19. X. Wang and X. Zhong, "A High-Order Shock-Fitting Non-Equilibrium Flow Solver for DNS of Strong Shock and Turbulence Interactions," Seventh International Conference on Computational Fluid Dynamics, Paper ICCFD7-2305, Big Island, Hawaii, July 9-13, 2012.
20. X. Wang and X. Zhong, "DNS of strong shock and turbulence interactions with thermochemical non-equilibrium effects," AIAA Paper 2012-3162, 2012.
21. X. Wang and X. Zhong, "Thermochemical non-equilibrium effects on passive control of hypersonic boundary-layer transition using regular porous coating," AIAA Paper 2011-3256, 2012.
22. C. Mortensen and X. Zhong, "High-Order Shock-Fitting Method for Hypersonic Flow with Graphite Ablation and Boundary Layer Stability", AIAA Paper 2012-3150, June 2012.
23. X. Wang and X. Zhong, "Effect of compressibility on strong shock and turbulence interactions," AIAA Paper 2012-1243, 2012.

4. AST070022

24. Barai, P., Proga, D., & Nagamine, K. 2011, MNRAS, 418, 591, Smoothed particle hydro-dynamics simulations of black hole accretion: a step to model black hole feedback in galaxies
25. -. 2012, MNRAS, 424, 728, Multiphase, non-spherical gas accretion on to a black hole
26. -. 2011, MNRAS, 410, 2579, Multicomponent and variable velocity galactic outflow in cosmological hydrodynamic simulations
27. . 2012, MNRAS, 419, 1280, On the inconsistency between the estimates of cosmic star formation rate and stellar mass density of high-redshift galaxies

28. Jaacks, J., Choi, J.-H., Nagamine, K., Thompson, R., & Varghese, S. 2012a, MNRAS, 420, 1606, Steep faint-end slopes of galaxy mass and luminosity functions at z _ 6 and the implications for reionization
29. Jaacks, J., Nagamine, K., & Choi, J.-H. 2012b, ArXiv e-prints, Duty Cycle and the Increasing Star Formation History of z ≥6 Galaxies
30. Niino, Y., Choi, J.-H., Kobayashi, M. A. R., Nagamine, K., Totani, T., & Zhang, B. 2011, ApJ, 726, 88, Luminosity Distribution of Gamma-ray Burst Host Galaxies at Redshift z = 1 in Cosmological Smoothed Particle Hydrodynamic Simulations: Implications for the Metallicity Dependence of GRBs
31. Thompson, R. & Nagamine, K. 2012, MNRAS, 419, 3560, Pairwise velocities of dark matter haloes: a test for the _ cold dark matter model using the bullet cluster
32. Virgili, F. J., Zhang, B., Nagamine, K., & Choi, J.-H. 2011, MNRAS, 417, 3025, Gamma-ray burst rate: high-redshift excess and its possible origins
33. Yajima, H., Choi, J.-H., & Nagamine, K. 2011a, ArXiv e-prints, Effect of radiative transfer on damped Lyman-alpha and Lyman limit systems in cosmological SPH simulations
34. -. 2011b, MNRAS, 412, 411, Escape fraction of ionizing photons from high-redshift galaxies in cosmological SPH simulations

5. AST080005

35. Mock Catalogs for UHECR Studies, Berlind, A., et al., 2011, arXiv:1112.4188
36. Large-scale bias and e_cient generation of initial conditions for nonlocal primordial non-Gaussianity, Scoccimarro, R. et al, 2012, Physical Review D, vol. 85, Issue 8, id. 083002
37. The Extreme Small Scales: Do Satellite Galaxies Trace Dark Matter? Watson, D., et al. 2012. ApJ, 749, 1
38. The clustering of galaxies at z 0.5 in the SDSS-III Data Release 9 BOSS-CMASS sample: a test for the LCDM cosmology, Nuza, S., et al. 2012, MNRAS submitted. arXiv:1202.6057
39. The clustering of galaxies in the SDSS-III Baryon Oscillation Spectroscopic Survey: a large sample of mock galaxy catalogues, Manera, M, 2012, MNRAS accepted. arXiv:1203.6609
40. Halo Sampling, Local Bias and Loop Corrections, Chuen Chan, K., Scoccimarro, R., 2012, arXiv:1204.5770
41. Measuring D A and H at z=0.35 from the SDSS DR7 LRGs using baryon acoustic oscillations, Xu, X., 2012, MNRAS submitted. arXiv:1206.6732
42. MPTbreeze: A fast renormalized perturbative scheme, Crocce, M., et al., 2012, MNRAS submitted. arXiv:1207.1465
43. External Members using LasDamas data: The public mock galaxy catalogs have been used as a basis for many additional works. To date, there are over 43 such publications either in print of pending. We know of several additional papers (at least 5) currently in preparation that are not included in this count.

6. AST090001

44. “Galactic Coronae in the Intracluster Environment: Semi-confinedStellar-feedback-driven Outflows,” Lu, Z., & Wang, Q. D., 2011, MNRAS, 413, 347

7. AST100001

45. W. Zhang, L. Howell, A. Almgren, A. Burrows, & J. Bell, ”CASTRO: A New Compressible Astrophysical Solver. II. Gray Radiation Hydrodynamics,” Astrophys. J. Suppl., 196, 20, 2011 (arXiv:1105.2466).
46. W. Zhang, L. Howell, A. Almgren, A. Burrows, J.C. Dolence, & J. Bell, ”CASTRO: A New Compressible Astrophysical Solver. III. Multigroup Radiation Hydrodynamics,” accepted to Astrophys. J. (arXiv:1207.3845).
47. J. Nordhaus, T. Brandt, A. Burrows, & A. Almgren, ”The Hydrodynamic Origin of Neutron Star Kicks,” M.N.R.A.S., 423, 1805, 2012 (arXiv:1112.3342).
48. E. Abdikamalov, A. Burrows, C.D. Ott, F. Loeffler, E. O’Connor, J.C. Dolence, & E. Schnetter, ”A New Monte Carlo Method for Time-Dependent Neutrino Radiation Transport,” Astrophys. J., 755, 111, 2012 (arXiv:1203.2915).
49. Adam Burrows, Josh Dolence, & Jeremiah Murphy, ”An Investigation into the Character of Pre-Explosion Core-Collapse Supernova Shock Motion,” 2012, accepted to Astrophys. J.,arXiv:1204.3088.
50. J.W. Murphy, J.C. Dolence, & A. Burrows, ”The Dominance of Neutrino-Driven Convection in Core-Collapse Supernovae,” submitted to Astrophys. J., 2012 (arXiv:1205.3491).
51. Adam Burrows, ”Thoughts on Core-Collapse Supernova Theory,” submitted to Rev. Mod. Phys., 2012.
52. Ott, C.D., O’Connor, E., Peng, F., Reisswig, C., Sperhake, U., Schnetter, E.,Abdikamalov, E., Diener, P., Loffler, F., Hawke, I., Meakin, C.A., & Burrows, A., ”New open-source approaches to the modeling of stellar collapse and the formation of black holes,” Astrophys. & Space Sci., 336, 151, 2011.
53. J.C. Dolence, A. Burrows, & J.W. Murphy, ”Dimensional Dependence of the Hydrodynamics in Core-Collapse Supernovae,” submitted to the Astrophysical Journal, 2012. 18.2

54. Adam Burrows, ”Multi-Dimensional Core-Collapse Supernova Explosions,” to appear in the proceedings of the 11th International Symposium on the Origin of Matter and Evolution of Galaxies (OMEG11)), held at RIKEN, Tokyo, Japan on Nov. 14 - Nov. 17, 2011 (AIP Conference series), eds. K. Nakamura, T. Kajino, and S. Kubono.

8. AST100005

55. M. Rempel, “Numerical Models of sunspot formation and fine structure”, 2012, Philosophical Transactions of the Royal Society A, vol. 370, issue 1970, pp. 3114--- 3128
56. M. Rempel, “Numerical Sunspot Models: Robustness of Photospheric Velocity and Magnetic Field Structure”, 2012, ApJ 750, 62
57. M. Rempel, “Subsurface magnetic field and flow structure of simulated sunspots”, 2011, ApJ, 740, 15
58. M. Rempel & R. Schlichenmaier, “Sunspot Modeling: From Simplified Models to Radiative MHD Simulations”, 2011, Living Reviews in Solar Physics, vol. 8, no. 3
59. A. Kilcik, V.B. Yurchyshyn, M. Rempel, V. Abramenko, R. Kitai, P.R. Goode, W. Cao & H. Watanabe, “Properties of Umbral Dots as Measured from the New Solar Telescope Data and MHD Simulations”, 2012, ApJ 745, 163
60. D.C. Braun, A.C. Birch, M. Rempel, & T.L. Duvall, “Helioseismology of a Realistic Magnetoconvective Sunspot Simulation”, 2012, ApJ 744, 77
61. L. Bharti, M. Schüssler & M. Rempel, “Can overturning motions in penumbral filaments be detected?”, 2011, ApJ, 739, 35
62. M. Rempel & M.C.M. Cheung, “Simulation of a full active region life cycle”, 2012, ApJ, in preparation
63. M.C.M. Cheung & H. Isobe, “Flux Emergence (Theory)”, 2013, Living Reviews in Solar Physics, invited review paper in preparation.

9. AST100035

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65. Gargat´e, L., Spitkovsky, A. 2012, Ion acceleration in non-relativistic astrophysical shocks, ApJ, 744, 67
66. Kugland, N., Ryutov, D., Chang, P.-Y., Drake, R. P., Fiksel, G., Froula, D. H., Glenzer, S. H., Gregori, G., Grosskopf, M., Koenig, M., Kuramitsu, Y., Kuranz, C., Levy, M. C., Liang, E., Meinecke, J., Miniati, F., Morita, T., Pelka, A., Plechaty, C., Presura, R., Ravasio, A., Remington, B. A., Reville, B., Ross, J. S., Sakawa, Y., Spitkovsky, A., Takabe, H. & Park, H.- S. 2012, “Self-organized electromagnetic field structures in laser-produced counter-streaming plasmas,” Nature Physics, 10.1038/nphys2434
67. Riquelme, M.A., Spitkovsky, A., Electron Injection by Whistler Waves in Non-relativistic Shocks, ApJ, 733, 63, 2011
68. Caprioli, D., Spitkovsky, A., 2012, Injection into Fermi acceleration process in collisionless shocks, in preparation Conference presentations and proceedings
69. Caprioli, D., “Fermi Acceleration in Supernova Remnant Shocks,” arXiv: 1210.0914; contributed talk at the 5th International Symposium on High-Energy Gamma-Ray Astronomy, Heidelberg (Germany), July 2012
70. Riquelme, M. & Spitkovsky, A. 2012, “Electron injection by whistler waves in non-relativistic shocks,” AIP Conf. Proc., 1439, 182
71. Gedalin, M. & Spitkovsky, A. 2012, “Heliospheric and astrophysical shocks: Common features and differences,” AIP Conf. Proc., 1439, 172
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74. Caprioli, D., Contributed talk at the 2nd Sant Cugat Forum in Astrophysics: Cosmic ray induced phenomenology in star-forming environments, Barcelona (Spain), April 2012
75. Gargat´e, L., Spitkovsky, A., Hybrid codes: numerical properties and applications to astrophysical shock scenarios, 22nd ICNSP, Long Branch, NJ, 2011
76. Gargat´e, L., Spitkovsky, A., Park, H.-S., Kugland, N. L., Ross, J. S., Remington, B. A., Pollaine, S. M., Ryutov, D. D., Gregori, G., Sakawa, Y., Kuramitsu, Y., Takabe, H., Froula, D. H., Fiksel, G., Miniati, F., Koenig, M., Ravasio, A., Woolsey, N., & Grosskopf, M, PIC simulations of laser-induced collisionless shocks in the laboratory, 11th IPELS meeting, Whistler (Canada), July 2011
77. Spitkovsky, A., Colloquium at Northwestern University, Feb 2012

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78. Law, K.-H., & Gordon, K. D. 2012, Key Insights on Nearby Galaxies Meeting Abstracts
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11. AST11050

81. Zalucha, A. M., and T. I. Michaels (2012), “A 3D general circulation model for Pluto and Triton with fixed volatile abundance and simplified surface forcing,” Icarus, submitted.

12. AST110051

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83. Krueger, B. K., Calder, A. C., Zingale, M., Almgren, A. S., Bell, J. B., Nonaka, A., \Low Mach Number Simulations of Classical Novae" American Astronomical Society, Meeting #219, #211.04
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89. Michael, S., Steiman-Cameron, T., Durisen, R. H., Boley, A. (2012) Convergence Studies of Mass Transport in Disks with Gravitational Instabilities I: The Constant Cooling Time Case. ApJ, 746, 98
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14. AST120006

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95. Krumholz, M. R., & Thompson, T. A. 2012b, \Numerical Simulations of Radiatively-Driven Dusty Winds", The Astrophysical Journal, in preparation

15. AST120010

96. Sironi, L. 2012, Particle Acceleration by Collision-Driven Reconnection in Astrophysical Jets, in prep.
97. Sironi, L., Spitkovsky, A. & Arons, J. 2012, The Maximum Energy of Accelerated Particles in Relativistic Shocks, in prep.
98. Sironi, L. & Spitkovsky, A. 2012, Particle-in-Cell Simulations of Shock-Driven Reconnection in Relativistic Striped Winds, Comput. Sci. Disc. 5, 014014
99. Narayan, R., □Ozel, F. & Sironi, L. 2012, Radio Synchrotron Emission from a Bow Shock around the Gas Cloud G2 Heading toward the Galactic Center, ApJL, 757, L20

16. ATM060012

100. Maliawco Jr., R.J., G.M. McFarquhar, and B.F. Jewett, 2012: An ensemble approach to examining the role of cloud condensation nuclei on the evolution of idealized tropical cyclones. Amer. Meteor. Soc. 30th Conf. Hurricanes Trop. Meteor., Ponte Vedra Beach, FL, 15-20 April 2012.

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17. ATM070010

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18. ATM090047

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19. ATM090060

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622. J. Li and E. Tajkhorshid. Molecular Insight for the Ion-coupling Mechanism of Secondary Active Transporters. Gordon Research Conference: Membrane Transport Proteins 2012. Les Diablrets, Switzerland.
623. J. Li and E. Tajkhorshid. Computational Observation of State Transition in LeuT-fold Transporters. (Oral Presentation & Best Talk Award) 9th Annual Biophysics and Computational Biology Symposium 2011. Urbana, IL.
624. J. Li and E. Tajkhorshid. Molecular Insight of State Transition and Ion-coupling in LeuT-fold Transporters. Biophysical Society 56th Annual Meeting 2012. San Diego, CA.
625. W. Han and E. Tajkhorshid. Transient Water Chains Connecting the Cytoplasmic and Extracellular Glutamate Gates in CLC. (Oral Presentation) Biophysical Society 56th Annual Meeting 2012. San Diego, CA.
626. P. Mahinthichaichan, J. Hemp, R.B. Gennis, and E. Tajkhorshid. Probing Gas Diffusion Pathways in Cytochrome C Oxidase. Biophysical Society 56th Annual Meeting 2012. San Diego, CA.
627. G. Enkavi and E. Tajkhorshid. Transport Cycle of Mitochondrial Carriers from Internal Symmetries. Biophysical Society 56th Annual Meeting 2012. San Diego, CA.
628. J. L. Baylon and E. Tajkhorshid. Capturing Insertion and Dynamics of Membrane-bound Cytochrome P450 3A4 using a Novel Membrane Mimetic Model. Biophysical Society 56th Annual Meeting 2012. San Diego, CA.
629. J. Vermaas and E. Tajkhorshid. Conformational Dynamics of Membrane-bound _-synuclein in a Highly Mobile Membrane Mimetic. Biophysical Society 56th Annual Meeting 2012. San Diego, CA.
630. T. Jiang, M. Spies, and E. Tajkhorshid. Characterizing an Intermediate State between Inactive and Active States of RecA. Biophysical Society 56th Annual Meeting 2012. San Diego, CA.
631. C. G. Mayne, J. A. Katzenellenbogen, and E. Tajkhorshid. Characterizing Structural and Dynamical Impacts of Agonist- and Antagonist-stabilized Mutants of the Estrogen Receptor. Biophysical Society 56th Annual Meeting 2012. San Diego, CA.
632. E. Tajkhorshid. Capturing Functional Motion of Membrane Transporters at an Atomic Resolution (2011) Department of Physiology, School of Medicine, Johns Hopkins University, Baltimore, Maryland, USA.
633. E. Tajkhorshid. Capturing Functional Motion of Membrane Transporters at an Atomic Resolution with Large-Scale Molecular Dynamics Simulations (2011) Departments of Physics and Physiology, University of Montreal, Montreal, Quebec, Canada.
634. E. Tajkhorshid. Membrane Transporters - Molecular Machines Coupling Cellular Energy to Vectorial Transport Across the Membrane (2011) Rise of The Machines: Integration of experiment, simulation and theory for a mechanistic understanding of biomolecular machines, Telluride Science Research Center, Telluride, Colorado, USA.
635. E. Tajkhorshid. Dynamical View of Energy Coupling Mechanisms in Active Membrane Transporters (2012) Physics Colloquium, Department of Physics, Indiana University Purdue University Indianapolis, Indianapolis, Indiana, USA.
636. E. Tajkhorshid. Characterizing Functional Motions and Chemomechanical Coupling Mechanisms in Membrane Transporters (2012) Invited lecture at Gordon Research Conference on Protons and Membrane Reactions, Ventura, California, USA.
637. E. Tajkhorshid. Accelerating Membrane Insertion of Peripheral Proteins with a Novel Membrane Mimetic Model (2012) Invited Symposium at 56th Annual Meeting of the Biophysical Society, San Diego, California, USA.
638. E. Tajkhorshid. Capturing Functional Motions of Membrane Transporters at an Atomic Resolution (2012) Department of Physiology and Biophysics, Rosalind Franklin University of Medicine and Science, Chicago, Illinois, USA.
639. E. Tajkhorshid. Visualizing the Dynamics of the Alternating Access Mechanism in Membrane Transporters at Atomic Resolution (2012) Department of Structural and Chemical Biology, Mount Sinai School of Medicine, New York City, New York, USA.
640. E. Tajkhorshid. Developing an Atomistic, Highly Mobile Membrane Model (HMMM) and Its Wide Applications (2012) Frontiers in Membrane Protein Structural Dynamics Computational MiniSymposium, Gordon Center for Integrative Science, University of Chicago, Chicago, Illinois, USA.
641. E. Tajkhorshid. Characterizing Optimal Pathways for Large-Scale Conformational Changes of Membrane Transporters (2012) Frontiers in Membrane Protein Structural Dynamics, University of Chicago Gleacher Center, Chicago, Illinois, USA.
642. T. V. Pogorelov. Membranes as a Platform for Protein Activation: Capturing Dynamics of Lipid Bilayers and Protein-membrane Interactions. (2011) Department of Chemistry, Sapienza University of Rome, Italy.

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645. T. V. Pogorelov. Computational Chemistry: A Brief Introduction with Research Examples. Invited lecture at ”Physics of Life Summer School for High School Teachers” (2011) NSF Center for Physics of Living Cells, University of Illinois at Urbana-Champaign, Urbana, IL.
646. Y. Z. Ohkubo. Enhanced Sampling of Specific Lipid Binding Sites of Membrane-Anchoring Proteins by a Highly Mobile Membrane Mimetic (HMMM) Model. (2011) Institute of Molecular and Cellular Biosciences, University of Tokyo, Japan.
647. Y. Z. Ohkubo. Spontaneous Binding and Insertion of Membrane-anchoring Proteins Captured by a Novel Membrane-mimetic System. (2011) Quantitative Biology Center, RIKEN Advanced Institute for Computational Science, Kobe, Japan.
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662. Numerical Modeling of the Solar Wind Flow with Observational Boundary Conditions, 11th Annual Astrophysics Conference, Palm Springs, CA, March 19-23, 2012. (Invited).
663. Unsteady Processes in the Vicinity of the Heliopause, 13th International Solar Wind Conference, 18-22 June, 2012, Big Island, HI.

664. Modeling Solar Wind Flow with the Multi-Scale Fluid-Kinetic Simulation Suite, 7th International Conference on Numerical Modeling of Space Plasma Flows, 24-29 June, 2012, Big Island, HI.
665. Modeling Heliosheath Flow with Observational Boundary Conditions, 39th COSPAR Scientific Assembly, 14-22 July, 2012, Mysore, India.
666. Solar Wind Behavior at Voyager Spacecraft from the Simulation Perspective, Voyager Science Steering Group Meeting, 4-5 September, 2012, Pasadena, CA.
667. Modeling CMEs from the Sun to the Earth Orbit, 2nd In-situ Heliospheric Science Conference, September 18-20, 2012, Laurel, MD.
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680. Zhengping Jiang, Yeqing Lu, Yaohua Tan, Yu He, Michael Povoloskyi, Tillmann Kubis, Alan Seabaugh, Patrick Fay, Gerhard Klimeck "Atomistic Simulation of GaSb/InAs Tunneling Field Effect Transistor" oral presentation in TECHCON ,September 10-11 2012, Austin TX
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779. Trampedach, R., Invited talk, “Solar and stellar modelling: From 1D to 3D”, at ‘HELAS 5: The Modern Era of Helio- and Asteroseismology’, Obergurgl, Austria, 21 May 2012.
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787. Brun, A.S., Invited talk, “On stellar cycles”, in Proc. IAU Symp. 286, ‘Comparative Magnetic Minima: Characterizing Quiet Times in the Sun and Stars’, Mendosa, Argentina, Oct 2011, in press.
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795. Miesch, M.S., Talk, “Self-organization in convective dynamos”, IUGG General Assembly, Melbourne, Australia, 4 July 2011.
796. Miesch, M.S., Co-organizer and presenter, in ‘Working Group on Bridging the Great Divide: Linking the Solar Dynamo to the Dynamic Heliosphere’, 2012 SHINE Workshop, Snowmass, CO, 11 July 2011.
797. Miesch, M.S., Invited talk, “Exploring the dynamo from all angles”, in ‘The Sun 360, Stereo-4/SDO-2/ SOHO-25 Workshop’, Kiel, Germany, 29 July 2011.
798. Miesch, M.S., Plenary talk, “Solar convection and dynamo”, NASA Heliophysics Summer School, Boulder, CO, 2 Aug 2011.
799. Miesch, M.S., Invited talk, “Convective Babcock-Leighton dynamo models”, Session SH22: ‘The Sun and the Heliosphere During the Solar Cycle 23/24 Minimum’, AGU Meeting, San Francisco, 2 Dec 2011.
800. Miesch, M.S., Four invited talks, on theme of “A closer look at the mysteries of the solar dynamo”, as part of the ‘Elementary Conversations About Solar-Terrestrial and Space Physics Series’, High Altitude Observatory, NCAR, Boulder, CO, 9 Mar to 11 May 2012.
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808. Toomre, J., Invited seminar, “Touching the inside of a convecting star and its magnetic dynamo”, Mathematics Dept., Univ. Waikato, Hamilton, New Zealand, 27 Jan 2012.
809. Toomre, J., Invited colloquium, “Probing the inside of a convecting star and its magnetism”, Mount Stromlo Observatory, Research School of Astronomy & Astrophysics, Australian National University, Canberra, Australia, 21 Feb 2012.
810. Toomre, J., Invited colloquium, “Joys of stellar convection and magnetism”, Dept. Physics, University of Sydney, Sydney, Australia, 24 Feb 2012.
811. Toomre, J., Invited colloquium, “Joys of convection and magnetism in stars”, South African Astronomical Observatory, Cape Town, South Africa, 22 Mar 2012.
812. Toomre, J., Augustson, K.C., Brown, B.P., Browning, M.K., Brun, A.S., Featherstone, N.A. & Miesch, M.S., 2012, “New era in 3-D modeling of convection and magnetic dynamos in stellar envelopes and cores”, in ‘61st Fujihara Seminar: Progress in Solar/Stellar Physics with Helio and Asteroseismology’, ASP Conf. Ser., in press.
813. Weber, M., Fan, Y. & Miesch, M.S., 2011, “The rise of active region flux tubes in the turbulent solar convective envelope”, Astrophys. J., 741:11 (14pp).
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815. Augustson, K., Brown, B.P., Brun, A.S., Miesch, M.S. & Toomre, J., 2012a, “Convection and differential rotation in F-type stars”, Astrophys. J., in press. [Copy provided as Appendix I]
816. Augustson, K., Brown, B.P., Brun, A.S., Miesch, M.S. & Toomre, J., 2012b, “Global shear instabilities driving by rotating convection in F-type stars”, Astrophys. J., to be submitted.
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821. Bonaca, A., Basu, S., Tanner, J. D.,..., Trampedach, R., et al., 2012, "An asteroseismic calibration of convection in stars", Astrophys. J., submitted.
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826. Browning, M.K., 2011, "Differential rotation and magnetism in simulations of fully convective stars", Proc. IAU Symposium 271, 'Astrophysical Dynamics: From Galaxies to Stars', Nice, France, 69–77 .
827. Browning, M.K., Invited talk, "Global MHD simulations of stellar dynamos and the ingredients for large-scale field organization", Proc. IAU Symp. 286, 'Comparative Magnetic Minima', Mendoza, Argentina, Oct 2011, in press.
828. Browning, M.K., Invited talk, "Effects of magnetism on stellar evolution", in program on 'The impact of asteroseismology across stellar astrophysics, KITP, UC Santa Barbara, Oct 2011.
829. Browning, M.K., Invited talk, "Ingredients for spatial and temporal order in global convective dynamo simulations", Royal Astronomical Society (specialist meeting on 'Mean Field Electrodynamics and Large-Scale Cosmic Magnetic Fields: Present Problems and Future Trends'), London, Feb 2012.
830. Browning, M.K., Invited talk, "Convection and magnetism in stars: puzzles and perspectives", Space Telescope Science Institute Colloquium, Apr 2012.
831. Browning, M.K., Invited talk, "Simulations of convection and magnetism in stars", Applied Mathematics department, Univ. Newcastle, UK, Apr 2012.
832. Browning, M.K., Invited talk, "Differential rotation on low-mass stars and its quenching by magnetic fields", Proc. 17th Cambridge Workshop on Cool Stars, Stellar Systems and the Sun, Barcelona, Spain, July 2012, submitted.
833. Collet, R., Hayek, W., Asplund, M., Nordlund, A, Trampedach, R. & Gudiksen, B., 2011, "Three-dimensional surface convection simulations of metal-poor stars. The effect of scattering on the photospheric temperature stratification, Astron. Astrophys., 528, A32 (12pp).
834. Featherstone, N.A., 2011, "Exploring convection and dynamos in the cores and envelopes of stars", Ph.D. thesis, University of Colorado, 174pp.
835. Featherstone, N.A., Browning, M.K., Brun, A.S. & Toomre, J., 2011, "Exploring the deep convection and magnetism of A-type stars", presentation at APS Division of Plasma Physics 53rd Meeting, Salt Lake City, UT.
836. Featherstone, N.A. & Miesch, M.S., 2012, "On the maintenance of meridional circulation and differential rotation in the Sun", presentation at Amer. Astron. Soc. 220nd Meeting, Anchorage, AK.
837. Mathur, S., Hekker, S., Trampedach, R., et al., 2011, "Characteristics of granulation and their correlation with the stellar properties in red giants observed by the Kepler mission", Astrophys. J., 741 (2), 119.
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1004. Sperhake, U., Black holes in D dimensions, Invited talk, 13th Marcel Grossmann Metting, Jul 2012, Stockholm, Sweden
1005. Cardoso, V., Dynamical black holes: beyond Einstein, Invited plenary talk, DECI Minisymposium, Workshop on State of the Art in Scientific and Parallel Computing, Jun 2012, Helsinki, Finland
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1007. Berti, E., Astrophysical tests of general relativity and black hole bombs, Invited talk: NEB 15 – Recent Developments in Gravity, Jun 2012, Chania, Greece
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G XSEDE Citation Report

Content for this appendix is pending the publication and subsequent citation of a research paper on the XSEDE project. XSEDE allocated users will be requested to cite this paper in their publications, thus enabling a more comprehensive analysis of the science impact of the XSEDE project.

H XSEDE EOT Event Details

Type	Title	Location	Date(s)	Hours	Number of Participants	Number of Under-represented people	Method	Funding Sources
webinar	Research Methodologies: Involvement in Scholarly Activities, Publishing and Timelines - Dr. M. Brian Blake	online	10/1/12	1	14	11	S	XSEDE
webinar	Safe CO2 Storage: Developing efficient models of underground fluid flow - Paul Delgado & Dr. Vinod Kumar	online	10/10/12	1	11	9	S	XSEDE
webinar	Mathematica in serial and parallel - Troy Schaudt, Wolfram Research, Inc, Academic Key Account Manager	online	10/22/12	1	15	11	S	XSEDE
webinar	MATLAB in serial and parallel - Gerardo Hernandez Correa, MathWorks Engineer	online	11/5/12	1	15	10	S	XSEDE
webinar	Statistics of functional brain networks - Manjari Narayan & Dr. Genevera Allen	online	11/7/12	1	50 (40 students from UT PanAm watched as a group)	44	s	XSEDE
Conference	National Organization of Black Chemist and Chemical Engineers (NOBBChe)	Washington DC	9/26/12	1 day	1,500	1,400	In-Person (Poster)	XSEDE
Conference	SREB The Compact for Faculty Diversity Institute on Teaching & Mentoring	Tampa, FL	10/25 – 10/27/2012	3 days	900	900	In-Person Exhibit Table	XSEDE
Conference	American Indian Science and Engineering Society Annual Mtg	Anchorage, AL	10/31 – 11/03/2012	4 days	1,800	1,700	Faculty Presentation	XSEDE
Conference	Virginia State University	Petersburg, VA	12/12/2012	1 day	9	9	In-Person	XSEDE
Conference talk	Oklahoma Supercomputing Symposium	University of Oklahoma, Norman, OK	10/2 - 10/3/2012	1	261		S	XSEDE, OK EPSCOR
Conference talks	Undergraduate computational science programs; XSEDE Education Program	CASC Meeting, Washington, DC	10/4/2012	4	100		S	
Workshop	Integrating Computational Science into the Curriculum	Central State University,	10/16/2012	6	19	19	S	XSEDE

		Wilberforce OH						
Workshop	Integrating Computational Science into the Curriculum	Sinte Gleska University, Mission, SD	10/12/2012	7	15	15	S	XSEDE
Workshop	Introducing Computational Science in the Curriculum	SC12, Salt Lake City, UT	11/11/2012	3	45		S	SC12, XSEDE
Workshop	LittleFe Build	SC12, Salt Lake City, UT	11/12/2012	12	41		S	SC12, XSEDE
Workshop	Computational thinking workshop	Monash University, Melbourne Australia	10/5/2012-10/11/2012	24	300 students 10 faculty		S	Monash University, XSEDE
Workshop	Computational Thinking Train the Trainer workshop	Pisgah Astronomical Research Institute, Rosman, NC	10-17-10/19/2012	14	22		S	XSEDE, Computing Matters NSF Grant
Conference talks	New Vistas in Computational Thinking: The Power and the Peril	Univ. Mary Washington	11/5/2012		15		S	XSEDE
Campus Visit	Computational science program	Durham Tech, Durham, NC	12/6/2012	3	3		S	XSEDE
Workshop	Computational thinking	New university in San Jose Costa Rico	12/15/2012	12	12		S	Pro bono
Workshop	Computational thinking	Univ. Mary Washington	12/17-12/18/2012	16	22		S	University XSEDE
Campus Visit	Integrating Computational Science into the Curriculum	Central State University, Wilberforce OH	12/16/2012	6	15		S	XSEDE
webinar	Research Methodologies: Involvement in Scholarly Activities, Publishing and Timelines - Dr. M. Brian Blake	online	10/1/12	1	14	11	S	XSEDE
webinar	Safe CO2 Storage: Developing efficient models of underground fluid flow - Paul Delgado & Dr. Vinod Kumar	online	10/10/12	1	11	9	S	XSEDE
webinar	Mathematica in serial and parallel - Troy Schaudt, Wolfram Research, Inc, Academic Key Account Manager	online	10/22/12	1	15	11	S	XSEDE
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